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Fundamentals and Applications
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Fundamentals and Applications

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Edited by:
E. Oñate
Universitat Politècnica de Catalunya, Spain

D.R.J. Owen
Swansea University, United Kingdom

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This volume contains the full papers presented at the II International Conference on Particle-based Methods (PARTICLES 2011), Barcelona, Spain, October 26-28, 2011. The previous conference on these series was held in Barcelona on 25-27 November 2009 and attracted some 150 participants.

PARTICLES 2011 addressed both the fundamental basis and the applicability of state of the art particle-based computational methods that can be effectively used for solving a variety of problems in engineering and applied sciences. The applications of the particle-based methods presented in the conference covered the analysis of geo-mechanical and mining problems, industrial forming processes, fluid-structure interaction problems accounting for free surface flow effects in civil and marine engineering (water streams acting on constructions, wave loads in harbours and marine structures, ship hydrodynamics, etc.), multi-fracturing processes in impact situations, nano-micro-macroscopic effects in material science and bio-medical engineering, molecular dynamics, quantum mechanics problems, melting of polymers in fire situations and many others.

PARTICLES 2011 was also a forum for practitioners in the computational mechanics field to discuss recent advances and identify future research directions for particle-based methods.

Altogether about 180 lectures were presented, including 7 Plenary Lectures and 6 special Invited Sessions organized by recognized experts in targeted research areas of particle-based techniques.

This volume includes contributions sent directly from the authors. The editors can not accept responsibility for any inaccuracies, comments and opinions contained in the papers.

The organizers would like to thank all authors for submitting their contributions, as well as the supporting organizations for their help in making PARTICLES 2011 possible.

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Eugenio Oñate
Technical University of Catalunya (UPC)
Barcelona, Spain

Roger Owen
University of Wales
Swansea
United Kingdom
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PLENARY LECTURES
MOVING PARTICLE SIMULATION FOR FREE SURFACE AND MULTI-PHASE FLOWS

S. KOSHIZUKA*

* Department of Systems Innovation, School of Engineering
  The University of Tokyo
  7-3-1, Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan
  e-mail: koshizuka@sys.t.u-tokyo.ac.jp

Key words: MPS, Tsunami, Multi-Phase Flow, Phase Change.

Abstract. This document provides particle simulation for free surface and multi-phase flows using the MPS (Moving Particle Simulation) method.

1 INTRODUCTION

Particle simulation is fitted to complex motion of free surfaces and multi-phase interfaces. The MPS (Moving Particle Simulation) method [1] has been used and is being developed for free surface and multi-phase flows. A review paper was published in [2]. Tsunami invasion with floating objects is one of the important issues which were recognized in the large tsunami disaster in Japan on March 11, 2011. Severe accident analysis which accompanies complex phase change processes in nuclear reactors is another challenging subject.

2 FREE SURFACE FLOWS

2.1 Tsunami

Large-scale simulation is necessary for three-dimensional analysis of tsunami invasion. Figure 1 shows an example [3]. 6,300,300 particles were used for 1,000x600m area. The particle size was 1m. The inflow boundary condition with an inflow velocity of 10m/s was set at offshore. Real geometries, which are supplied by private companies and a government organization, can be converted to the input data of the particle simulation.

Explicit MPS methods [4, 5] have been proposed without solving the Poisson equation of pressure. The time step width $\Delta t$ in the explicit MPS method can be the same as that in the semi-implicit MPS method when the Mach number is 0.2 [5]. Thus, the calculation speed is much faster in the explicit MPS method. The calculation time of the explicit method obeys $O(N^{1.0})$, where $N$ represents the number of particles. In the semi-implicit method, the calculation time is $O(N^{1.5})$. Therefore, the explicit algorithm is to be much faster in a larger problem.

There were a lot of damages due to floating objects, such as ships moored in a port, on March 11. The particle simulation can easily be applied to such problems involving the interaction between fluid flow and floating rigid bodies [6].
2.2 Lifeboat

Free fall of a lifeboat was analyzed in three dimensions [7]. The acceleration should be kept low for the human safety when it drops onto the sea surface. The lifeboat was represented by particles of which the relative coordinates were fixed as a rigid body. The interaction between the fluid flow and the rigid body was considered. Figure 2 shows a calculation result with a skid angle of 30 degrees. Splashing from the sea surface is observed. The calculated acceleration agreed well with the experimental one.

![Figure 2: Dropping of a lifeboat onto the sea surface with a skid angle of 30 degrees](image)

3 MULTI-PHASE FLOWS

3.1 Basic Processes

Basic processes of two-phase flows have been solved by the MPS method: oscillation of a square droplet due to surface tension, single droplet breakup, jet breakup and single bubble rising [2]. These results were compared with analytical solution or experimental observation.

Bubble growth and departure from a heated wall in nucleate boiling of water was calculated at atmospheric pressure using the MAS-MAFL (Meshless Advection using Flow-directional Local-grid) method which enables us ALE (Arbitrary Lagrangian-Eulerian) approach in the meshless framework [8]. In nucleate boiling of water, we need to analyze thin boundary layers developing on the heated wall and the bubble surface. Small particles were located in the boundary layers and they were moved arbitrary to keep them inside the layers. Figure 3 shows the calculation result. We can see that the bubble expands due to the heat from the bottom wall and that the growth is terminated by the heat balance between boiling and condensation. The bubble radius is provided in Fig.4. The growth stops at around 7ms which agrees well with experimental results. The calculated heat transfer is also in good agreement with that of the experiment.
3.2 Applications

Liquid droplet impingement (LDI) is one of the principal mechanisms of the pipe wall thinning in nuclear power plants. Pressure wave propagation in a droplet was analyzed with an impinging velocity of 200 m/s and a droplet diameter of 50 μm (Fig. 5) [9, 10]. A compressible-incompressible unified algorithm was employed. We can find that high pressure appears when the droplet impinges on the wall surface and it propagates upward in the droplet. The calculated pressure agreed with those of the existing correlations.

When high temperature molten core is dropped into low temperature coolant, a vapor explosion may occur. The cause of the vapor explosions is rapid fragmentation of the molten material and subsequent increase of the heat transfer area between high and low temperature liquids. The MPS method was used to analyze single droplet fragmentation (Fig. 6) [11, 12]. Multiple water jets impinged onto a molten tin droplet, which caused sharp spikes on the droplet surface. This behavior agreed well with X-ray photographs taken in the fragmentation process.

The MPS method has been applied to various phenomena in severe accidents of nuclear
reactors: molten core-concrete interaction (MCCI), in-vessel retention (IVR), molten core spreading etc [2].

4 CONCLUSIONS

Particle simulation has been used for complex free surface flows, such as tsunami invasion to the coast and ship-water interaction. Basic processes of multi-phase flows are analyzed, such as droplet oscillation due to surface tension, droplet breakup, jet breakup, a rising bubble and nucleate boiling. Complex behaviors in severe accidents of nuclear reactors have been analyzed by the MPS method.

REFERENCES


DISCRETE MODELLING OF A ROCKFALL PROTECTIVE SYSTEM

K. Thoeni*, C. Lambert†, A. Giacomini* and S.W. Sloan*

*Centre for Geotechnical and Materials Modelling
The University of Newcastle
Callaghan, NSW 2308, Australia
http://www.newcastle.edu.au

†Department of Civil and Natural Resources Engineering
University of Canterbury
Christchurch 8140, New Zealand
http://www.civil.canterbury.ac.nz

Key words: DEM, YADE, Rockfall Protective System, Double-Twisted Hexagonal Mesh

Abstract. Metallic wire meshes are used worldwide for rockfall protective systems, such as rockfall net barriers and drapery meshes. Within different types of meshes, the double-twisted hexagonal mesh is commonly used. This paper focuses on the implementation and validation of a computational tool for the simulation of the behaviour of such meshes as a single part and as a component of a rockfall protective system. The discrete element method (DEM) is used to model the rockfall mesh and the impacting blocks. The open-source framework YADE has been extended in this context. Tensile tests of a plane net sheet subjected to a constant strain rate are used to calibrate the numerical model. Finally, the simulation of an impacting block on a horizontally spanned net is investigated where numerical results are compared to experimental results.

1 INTRODUCTION

Rockfalls pose a significant safety hazard for people and infrastructure which needs to be rigorously managed, not only when dealing with mountainous regions, but also in quarries and mines. It is almost impossible to prevent these phenomena. However, the installation of rockfall protective systems, such as rockfall net barriers and drapery meshes, is a common and effective way to reduce the hazard. The design of such structures is mostly based on empirical assumptions and, therefore, there is still a need to develop efficient numerical models in order to efficiently control the rockfall hazard. A principal component of these protection systems is the metallic wire mesh. The mesh can be installed in a more complex system as a rockfall barrier or directly installed on the slope,
as in the case of drapery mesh systems. Different types of meshes are currently available from rockfall barrier producers, with the double-twisted hexagonal mesh being the most commonly used (see Figure 1). This wire mesh is made by continuously twisting two wires to form hexagonal-shaped openings as shown in Figure 2(a).

Figure 1: Application of double-twisted hexagonal rockfall mesh in a mine in New South Wales, Australia.

Several approaches for modelling steel wire meshes in numerical simulations have been proposed in the literature, with the most common being the finite element method (FEM). The FEM has been used to simulate the impact of falling rocks against rockfall protection systems where the wire meshes have been modelled by using truss elements (see e.g. [4]), beam elements (see e.g. [3]), shell finite elements (see e.g. [10]) and special purpose finite elements (see e.g. [11]). The FEM is well established for dynamic modelling of non-linear geometries with complex mechanical and contact behaviour for continuum problems but, when dealing with discontinuous problems, computing time becomes a big issue especially if the failure of the wire mesh needs to be considered. Therefore, the discrete element method (DEM) is a good alternative since the method is particularly suitable for dynamic impact problems involving failure. In this work the open-source framework YADE [8, 12] has been extended to model the double twisted hexagonal wire mesh. For this purpose, a new material and the related contact laws for the double-twisted wire mesh have been implemented.

2 DISCRETE MODELLING OF THE WIRE MESH

Following an initial idea by [9], and later extended by [1, 2], the mesh is discretised by a set of spherical particles which are located at the physical nodes of the mesh. The positions of the particles and remote interactions (i.e. interactions between the particles exist without direct contact) are defined by the initial geometry of the mesh. Two dif-
ifferent remote interactions have been introduced to represent single and double-twisted wires. The constitutive relations proposed by [1] are used at the contact level to take the elastoplastic behaviour of the metallic wire mesh into account.

2.1 Remote interaction model and particle interaction

A nodal description of the wire mesh with remote interaction is used. As shown in Figure 2(b) particles are generated at the physical nodes of the mesh only. The wire itself is not discretised because interactions between particles exist without contact. In YADE the interactions are created by defining a interaction radius. Firstly, the particles are generated depending on the initial geometry of the mesh. Figure 2(a) shows a hexagon of the double twisted mesh with the requested dimensions to generate the mesh in YADE. Secondly, a simulation step is executed by defining a specific interaction radius. This simulation step initialises the interactions and creates the physical net. The generation of the mesh particles is done in a specific way in which double-twisted interactions are automatically identified. The algorithm always starts at the left lower corner of the mesh and generates a pair of particles which corresponds to a double-twist. Therefore, the number of the particles is used to identify if the interaction is a double-twisted or a single wire. For double-twisted interactions the following relation holds

$$|n_i - n_j| = 1$$ (1)

where \( n_i \) and \( n_j \) are the number of particle \( i \) and \( j \) respectively. However, not all interactions might be created by the initialisation step since only interactions between the same wire material are identified automatically. The interactions for the selvedge wire, which is used to edge the wire, has to be defined manually. The same applies if additional wires (or wire ropes) are used to strengthen the wire mesh.

(a) Basic hexagonal shape of the double-twisted wire mesh [5] with dimensions used in YADE.

(b) Particles and remote interaction model.

Figure 2: Shape and remote interaction model of the double-twisted hexagonal mesh.
2.2 Constitutive law

The constitutive relations proposed by [1] have been adapted in this work. However, the implementation in YADE does not follow the incremental formulation presented in [1]. The contact law is directly defined by a piece-wise linear force-displacement curve (e.g. Figure 4) which is derived from the stress-strain curve of a single wire. Figure 3 shows the stress-strain curve used for the simulation. The relation corresponds to the stress-strain curve used by [1].

![Figure 3: Piece-wise linear stress-strain curve used for the modelling of the steel wire.](image)

It should be mentioned that the current implementation for the constitutive behaviour was kept very general in YADE. In fact, there is no limitation on how many points are used to define the piece-wise linear stress-strain curve. Any piece-wise function can be used to represent the tensile behaviour of a wire and, therefore, additional wire or even wire ropes can easily be considered in the model.

The force-displacement relation for a double-twisted wire is derived from that of the single wire by introducing two local parameters \( \lambda_k \) and \( \lambda_c \) as shown by [1]. The parameter \( \lambda_k \) defines the initial stiffness of the double-twist, whereas \( \lambda_c \) takes the length reduction at failure into account. These parameters are then used to calibrate the numerical model. The implemented model considers tensile forces only. It is assumed that tensile forces are much higher than compressive forces because of the buckling effect. Therefore, the stiffness in the compression regime is set to zero. Furthermore, only normal forces and no shear forces are considered in the model. Unloading is considered by setting the corresponding stiffness equal to the initial elastic stiffness. The interaction breaks when its strain limit is reached. Figure 4 shows the basic behaviour of a single wire on a loading path with unloading and reloading.
3 CALIBRATION OF DISCRETE WIRE MODEL

The procedure presented in [2] is used to calibrate the two parameters used in the model. A tensile test of a plane net sheet of $0.5 \text{m} \times 1 \text{m}$ subjected to a constant strain rate is analysed. The net is fixed at the bottom while a constant strain rate is applied at the top as shown in Figure 5(a). The diameter of the wire used for the mesh is $2.7 \text{mm}$. The selvedge wire which is used to edge the mesh at its sides has a diameter of $3.4 \text{mm}$. The behaviour of both wires follows the stress-strain curve presented in the previous section. A mesh of the type $80 \text{mm} \times 100 \text{mm}$ is considered. The dimensions used for the generation of the mesh are $m_{os} = 80 \text{mm}$ and $a = b = 40 \text{mm}$.

No gravity is considered in this simulation since its influence on the tensile strength can be neglected. A displacement of $1.144 \cdot 10^{-3} \text{mm}$ is applied in each time step. The time step proposed by [2] is used. It is defined as

$$
\Delta t = \frac{1}{5} \sqrt{\frac{m}{2k_s}},
$$

where $m$ corresponds to the mass of a particle and $k_s$ is the elastic stiffness of the single wire. The mass of the type of mesh considered in the analysis is $1.42 \text{kg/m}^2$.

The influence of the two parameters $\lambda_k$ and $\lambda_\varepsilon$ is studied and shown in Figure 6 where the numerical results of this work are compared to the experimental results presented in [2]. As can be seen from Figure 6(b), a good approximation of the experimental curves is obtained with $\lambda_k = 0.73$ and $\lambda_\varepsilon = 0.47$.

4 SIMULATION OF IMPACT

The dynamic impact of a concrete block on a horizontal hexagonal mesh is analysed and compared to experimental results in order to investigate the contact behaviour of the wire mesh with a block. Experimental tests have been carried out at the laboratory of The Centre for Geotechnical and Materials Modelling at The University of Newcastle according to the experimental set up developed in [3]. In this study, a series of tests have been carried out by fixing a double-twisted hexagonal mesh at two sides of the testing
K. Thoeni, C. Lambert, A. Giacomini and S.W. Sloan

(a) Boundary conditions and discretisation for the tensile test.

(b) Deformed mesh and normal forces before failure ($\lambda_k = 0.73, \lambda_\varepsilon = 0.47$).

**Figure 5**: Tensile test of a plane net sheet subjected to a constant strain rate.

(a) Calibration of $\lambda_k$ with $\lambda_\varepsilon = 1.0$.

(b) Calibration of $\lambda_\varepsilon$ with $\lambda_k = 0.73$.

**Figure 6**: Calibration of the parameters $\lambda_\varepsilon$ and $\lambda_k$.

frame structure and then dropping concrete blocks on to the mesh from different heights. Figure 7(a) shows the experimental set up and the boundary conditions. The impacting concrete block, shaped according to the European Organisation for Technical Approval guidelines [7], has a mass of 44.5 kg and dimensions of 30 cm. The block was dropped from a dropping height of 0.5 m.

In the simulation, the block is represented by a clump generated by 1576 particles which have the same size as the particles used to represent the mesh (see Figure 7(b)). The mesh used for this example is the same as that used in the previous section where a sheet of 2 m $\times$ 2 m is considered. The contact forces between the block and the wire mesh are computed using the classical linear elastic-plastic law from [6], which is implemented in YADE [12]. A local friction angle of $\varphi = 30^\circ$ has been assumed.

In the numerical simulation, gravity is applied to the wire mesh and after it has reached equilibrium the block is released. The maximum deformation of the mesh after the impact
has been compared to the experimental measurements. The calculated deformation is 31 cm, whereas the deformation measured in the experimental tests varies between 32 cm and 38 cm. A very good agreement is thus observed. However, the behaviour of velocity and acceleration still needs to be analysed in order to fully validate the model.

(a) Experimental set up with concrete block and deformed mesh.

(b) Discrete model and deformed mesh with block clump.

Figure 7: Experimental test and numerical model for a block impacting on a horizontal spanned double-twisted wire mesh.
5 CONCLUSIONS

This paper presents a discrete wire mesh model currently implemented in the open-source framework YADE, which has the capability to model hexagonal double-twisted wire meshes. The application to rockfall protective systems has been investigated. However, only a very simple example is presented and further research is under way.

The current work is part of an ongoing research project with the objective to assess the rockfall hazard in open pit coal mines. The discrete model will be used to study rockfall trajectories and velocities at highwalls which are protected by double-twisted hexagonal meshes.

REFERENCES


MODELLING COHESIVE-FRICTIONAL PARTICULATE SOLIDS FOR BULK HANDLING APPLICATIONS

JOHN P. MORRISSEY, SUBHASH C. THAKUR, JIN SUN, JIAN-FEI CHEN AND JIN Y. OOI

Institute for Infrastructure and Environment
School of Engineering, The University of Edinburgh
The King's Buildings
Edinburgh EH9 3JL
Scotland, U.K
E-mail: J.Morrissey@ed.ac.uk

Key words: Cohesive Solid, Granular Material, Discrete Element Method (DEM), Contact Model, Adhesion.

Abstract. Many powders and particulate solids are cohesive in nature and the strength often exhibits dependence on the consolidation stress. As a result, the stress history in the material leading up to a handling scenario needs to be considered when evaluating its handleability. This paper outlines the development of a DEM contact model accounting for plasticity and adhesion force, which is shown to be suitable for modelling the stress history dependent cohesive strength. The model was used to simulate the confined consolidation and the subsequent unconfined loading of iron ore fines with particle sizes up to 1.18mm. The predicted flow function was found to be comparable to the experimental results.

1 INTRODUCTION

Powders and bulk solids are usually stored and handled in large quantities in many industries. Their constituent particles, varying from nano-particles to grains and ores, differ greatly in size and shape. One common issue for many of these materials is the storage and handling difficulties caused by cohesion. The cohesive strength of a bulk material depends on the consolidation stress it has experienced. As a result, the stress history in the material leading up to a handling scenario needs to be considered when evaluating its handling behaviour. For example, high storage stresses in a silo can lead to high cohesive strength of the stored solid, which may in turn cause blockages such as ratholing or arching near the outlet during discharge.

The discrete element method (DEM) has been extensively used to simulate the behaviour of granular materials. For cohesive solids, it is crucial that the stress history dependent behaviour is adequately captured. A number of contact models are available in several commercial DEM packages to simulate cohesive granular materials. These include the JKR model [1] and capillary force models [2,3]. However, DEM simulations with these models may not capture the stress history dependency behaviour observed in bulk solids.
The paper presents a relatively simple contact model that accounts for plasticity and adhesion forces for use in DEM computation. The predictions using this model for iron ore fines are presented and compared with experimental data.

2 EXPERIMENTAL BEHAVIOUR OF COHESIVE GRANULAR MATERIALS

The flowability of bulk solids, particularly fine grained ones, is greatly affected by the adhesive forces that act between the particles. These forces can be attributed to van der Waals, electrostatic, capillary or magnetic forces to name just a few possible sources and all are dependent on the separation distance of the particles. In moist bulk solids, the capillary forces tend to become the dominant adhesive force, while van der Waals forces become less influential as particle size increases past several microns.

The flowability of bulk solids is usually measured using the flow function, which is the relationship between the unconfined yield strength (σc) and the consolidation stress (σ1). An iron ore fines provided by the Swedish company LKAB was used as the test material in this study to evaluate the capability of the proposed contact model. The flow behaviour was tested physically as described below.

2.1 Test Material

Iron ore fines are the finer fractions (< 6.3mm) that are broken off the main iron ore pellets during handling or storage. The iron ore fines used in this study are from LKAB Direct Reduction (KPRS) pellets and contain particles up to 1.18mm. The material had a bulk density of 2300 kg/m3 and solid density of 3700 kg/m3. The behaviour of the iron ore fines is expected to be affected by both the moisture content and the temperature of the sample. Only the effect of moisture content is investigated here. The fines were evaluated at four different moisture content levels: dry (< 0.25%), 1%, 2% and 4%. The moisture content MC was measured by drying a sample in an oven at 105°C for 24 hours.

2.2 Test method

The unconfined stress-strain relationship of the iron ore fine was tested using the Edinburgh Powder Tester (EPT). The EPT is a semi-automated uniaxial tester (Fig. 1), in which the cohesive strength of a bulk solid is evaluated from an unconfined compression test of a material following a period of consolidation to a pre-defined stress level (σ1). After the removal of the consolidation stress the confining tube is slid off carefully and a vertical force is applied to the sample through the top platen until failure of the sample.

Both the confined and unconfined responses of the iron ore fines were measured. The EPT allows for the evaluation of the bulk compressibility of a material by measuring the height of the sample at incremental consolidation loads. The load is applied to the sample and the sample height is allowed time to stabilise. Once stabilised this is recorded as the consolidated height. Not only can the confined vertical stress-strain response be measured, but also the variation in bulk density during loading, provided the sample mass is known.

During the loading process, the force acting on the top platen, as well as its displacement, are recorded from which the unconfined stress-strain curve can be obtained. The unconfined yield strength (σc) is the maximum force recorded during the test. By repeating the
experiment for a range of consolidation stresses the flow function of a bulk solid can be obtained quickly.

2.3 Test results

Figure 2 shows the confined stress-strain curves for the iron ore fines at various moisture content levels. The corresponding bulk density variation is shown in figure 3. The results for the dry iron ore fines are not shown as they did not display any cohesive strength up to a consolidation stress of 100 kPa.

Figure 4 shows the unconfined stress-strain responses for 20, 40, 60 and 80 kPa consolidation (at MC=2%). All the curves show a hardening behaviour initially until failure occurs at the maximum unconfined strength; after that the curves descend, showing a softening behaviour. The unconfined strength increases with the consolidation stress.
Once the series of unconfined tests (3-5 tests at each consolidation stress) is complete the flow function can be plotted as the best fit line through the test data. The flow functions for iron ore fines at 2%, 4% and 7% are plotted in figure 5.

3 PARTICLE CONTACT CONSTITUTIVE MODEL

3.1 Visco-elasto-plastic adhesive contact model

A non-linear contact model that accounts for both elastic and plastic contact deformation and adhesion is proposed. The force-overlap \( f_{op} \)–\( \delta \) diagram for this model is shown in figure 6. The loading, unloading/re-loading and adhesive branches are represented by four parameters: the virgin loading parameter \( k_1 \), the unloading and reloading parameter \( k_2 \), and the adhesive parameter \( k_{adh} \) and the exponent \( n \). The shape of all the three branches is controlled by the parameter \( n \) – they all become linear when \( n=1 \). Furthermore, if \( k_1 \) is set to equal to \( k_2 \) the model is reduced to a linear elastic contact model. The normal contact force-overlap...
relationship can be mathematically expressed as in Equation 1.

The model reloads initially along the re-loading path \( k_2 \) and switches to the virgin loading path \( k_1 \) when the previous maximum loading force is reached. Unloading below the plastic overlap \( \delta_p \) (Fig. 6) results in the development of an attractive force until the maximum attractive force is reached at \(-k_{adh}\delta_{min}\). Further unloading past this point results in a reduction in both the normal overlap and the attractive force until separation occurs.

\[
f_{\text{hys}} = \begin{cases} k_1\delta^n & \text{if } k_2 (\delta^n - \delta_p^n) \geq k_1\delta^n \\ k_2 (\delta^n - \delta_p^n) & \text{if } k_4\delta^n > k_2 (\delta^n - \delta_p^n) > -k_{adh}\delta^n \\ -k_{adh}\delta^n & \text{if } -k_{adh}\delta^n \geq k_2 (\delta^n - \delta_p^n) \end{cases}
\]

(1)

### 3.2 DEM implementation

In this study a value of \( n=1 \) is used which reverts the contact model to a simple linear hysteretic spring contact model accounting for plastic contact deformation [4-10]. In this case Equation 1 is reduced to Equation 2. The adhesion force is linear to the contact deformation and the maximum adhesion force is determined by the stiffness parameters and the maximum normal overlap \( \delta_{max} \), which is recorded and updated over the contact lifetime.

\[
f_{\text{hys}} = \begin{cases} k_1\delta & \text{if } k_2 (\delta - \delta_0) \geq k_1\delta \\ k_2 (\delta - \delta_0) & \text{if } k_4\delta > k_2 (\delta - \delta_0) > -k_{adh}\delta \\ -k_{adh}\delta & \text{if } -k_{adh}\delta \geq k_2 (\delta - \delta_0) \end{cases}
\]

(2)

The tangential stiffness is calculated based on a constant stiffness \( k_T \), which is set to 2/7 of the normal loading stiffness \( k_1 \). The tangential force is calculated from the product of the tangential stiffness and the tangential displacement, subject to the friction limit according to the Coulomb’s law. This contact model has been implemented through the API in EDEM® v2.3, a commercial DEM code by DEM Solutions Ltd [11,12]. Custom contact properties are used to record the maximum normal overlaps for contacts.

The default EDEM rolling friction model is adopted in this study.

### 4 DEM SIMULATION SETUP & RESULTS

The iron ore fines with 2% moisture content were selected as the test material for comparison. A series of uniaxial compression simulations for the test material were conducted using the new contact model. Closely following the EPT physical test procedure, each simulation consisted of three stages – filling the cylindrical mould which formed the initial packing to be used, confined consolidation to the required stress level, followed by unloading, and finally unconfined compression of the sample to failure after the removal of the confining mould.

The details of the simulation setup and parameters are introduced in the next section followed by a discussion of the simulation results.
4.1 Numerical model parameters

A cylinder of 6.5mm radius was filled with 2,500 mono sized spherical particles at 1mm diameter. The random rainfall method was adopted to provide a random packing of particle with a coordination number $C \approx 4$. The height of the sample was determined by the filling process in each simulation and was approximately 3-4 times of the radius of the cylinder. Adhesion between particles is accounted for (i.e. with $k_{adh}$ set at an assumed value) in the filling process to allow for the development of a filled porosity similar to the experimental data. If $k_{adh}$ is set to zero, the filling process would produce a highly packed sample with its porosity much lower than the actual material. Large static and rolling friction values were also employed to account for the rough, non-spherical nature of the actual iron ore fines. Values of the parameters used in the simulations are listed in table 1. All parameters were kept constant throughout all simulations.

The cohesive contact model was only applied to particle-particle interactions. The particle-geometry interactions were modelled using the widely used simplified Hertz-Mindlin contact model with no adhesion[13].

The sample was loaded at an axial speed of 5mm/s (strain rate $\approx 0.2 s^{-1}$) during the confined consolidation stage and a lower speed of 2.5mm/s (strain rate $\approx 0.125 s^{-1}$) during the unconfined compression.

To ensure that all simulations share the same packing structure and loading path (to the required stress levels), the first two stages of filling and consolidation occur in one simulation to the maximum consolidation stress to be considered. Models at each intermediate consolidation stress level were extracted from this simulation and unloaded at the specified consolidation stress, before being loaded to failure as a separate simulation.

<table>
<thead>
<tr>
<th>Table 1 - Simulation Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Poisson's Ratio, $v$</strong></td>
</tr>
<tr>
<td><strong>Shear Modulus, G (Pa)</strong></td>
</tr>
<tr>
<td><strong>Young's Modulus, E (Pa)</strong></td>
</tr>
<tr>
<td><strong>Particle Radius, R (m)</strong></td>
</tr>
<tr>
<td><strong>Particle Density, $\rho$ (kg/m$^3$)</strong></td>
</tr>
<tr>
<td><strong>Loading Spring Stiffness, $k_1$ (N/m)</strong></td>
</tr>
<tr>
<td><strong>Unloading Spring Stiffness, $k_2$ (N/m)</strong></td>
</tr>
<tr>
<td><strong>Adhesive Parameter Stiffness, $k_{adh}$ (N/m)</strong></td>
</tr>
<tr>
<td><strong>Particle Static Friction, $P_{sf}$</strong></td>
</tr>
<tr>
<td><strong>Particle Rolling Friction, $P_{rf}$</strong></td>
</tr>
<tr>
<td><strong>Wall Friction, $W_f$</strong></td>
</tr>
<tr>
<td><strong>Base Friction, $B_f$</strong></td>
</tr>
<tr>
<td><strong>Simulation Time step (s)</strong></td>
</tr>
</tbody>
</table>

5 SIMULATION RESULTS & DISCUSSION

Figure 7 shows the simulated stress-strain curves for different confined consolidation stress levels. The test results for the iron ore fines at 2% MC are also shown for comparison. The error bars on the experiments represent the range of measured strains in the experiments at each consolidation stress level, for example at 20 kPa the strain varied between 0.165 and 0.2.
The DEM simulations are in a reasonable agreement with the experimental data. The 40 and 60 kPa stress-strain curves lay within the experimental variation at these stress levels, while the 80 kPa is fractionally outside the experimental variation. Only the 20 kPa simulation is significantly outside the experimental range by under-predicting the vertical strain. Whilst this simplified contact model has clearly captured some of the non-linear nature of the experimental data, it appeared to predict a bulk response that is too stiff at lower stresses and too soft at higher stresses. Using an exponent value $n$ greater than unity in Eq. 1 can be expected to address this issue.

Much of the non-linearity of the experimental data was related to the rearrangement of the constituent particles. The use of a high rolling friction together with the adhesive forces during filling allowed the simulation to obtain a similar porosity to the iron ore fines. The simulation result had a similar initial softer response that became stiffer as the deformation increased.

The DEM results are compared to the experimental results for bulk density in figure 8 which shows a good agreement in terms of the initial and the maximum consolidated bulk density. The simulated maximum bulk density is 2450 kg/m$^3$ at a consolidation stress of 80 kPa which is very close to 2440 kg/m$^3$ measured experimentally at the same stress level. The initial bulk density measured under 3 kPa of consolidation stress in the experiments was 1830 kg/m$^3$. The corresponding bulk density from the DEM simulation was 1880 kg/m$^3$. Again the error bars represent the range of bulk densities calculated experimentally at each consolidation stress.

The difference in the bulk density at the end of unloading may be explained by the lack of wall friction in the DEM simulation, allowing a greater elastic rebound of the particles compared to the experimental setup where the friction present between the sample and walls prevented such a rebound occurring. Including friction between particles and the confining cylinder should help to reduce this discrepancy. The issue could also be remedied by increasing the unloading stiffness $k_2$, but an unloading stiffness of at least an order of magnitude larger would be required and this would reduce the required computational time step and thus increase the total run time significantly.

The difference in the bulk densities at the intermediate stress levels between the
experimental result and the DEM simulation is likely due to the linear nature of the contact model used. A non-linear relationship, similar to that of the Hertzian contact, should provide a much closer match to the non-linear result seen in the experimental data.

The peak strength achieved in each of the simulations is plotted against the consolidation stress giving the flow function in Figure 9. The test results are also plotted for comparison. The flow function calculated from the DEM simulations displays a linear trend, which differs from the nonlinear trend of the test results.

The simulation results provide a closer match to the experimental data at the higher consolidation stresses of 60 & 80 kPa with a much larger deviation occurring at the lower stresses of 20 kPa and 40 kPa. The 80 kPa simulation is the only one that lies within the experimental scatter for unconfined strength and is the only simulation to match the experimental bulk density at that stress level.

Comparing the discrepancy between experiment and simulation, we note that the discrepancy in unconfined strength and bulk density increased in tandem, with the 20 kPa simulation being the furthest from the experimental values. A detailed comparison of the results is presented in table 2 and table 3 below.

**Table 2 – Predicted vs test unconfined yield strength (2% M.C.)**

<table>
<thead>
<tr>
<th>Consolidation Stress (kPa)</th>
<th>20</th>
<th>40</th>
<th>60</th>
<th>80</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test: average (kPa)</td>
<td>2.90</td>
<td>5.63</td>
<td>7.64</td>
<td>9.83</td>
</tr>
<tr>
<td>Test: COV</td>
<td>0.093</td>
<td>0.051</td>
<td>0.035</td>
<td>0.096</td>
</tr>
<tr>
<td>DEM Simulation (kPa)</td>
<td>2.1</td>
<td>4.4</td>
<td>6.9</td>
<td>9.6</td>
</tr>
<tr>
<td>% Difference</td>
<td>-27.6%</td>
<td>-21.8%</td>
<td>-9.7%</td>
<td>-2.3%</td>
</tr>
</tbody>
</table>

**Table 3 – Predicted vs test consolidated bulk density (2% M.C.)**

<table>
<thead>
<tr>
<th>Consolidation Stress (kPa)</th>
<th>20</th>
<th>40</th>
<th>60</th>
<th>80</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test: average (Kg/m³)</td>
<td>2250.62</td>
<td>2322.54</td>
<td>2400.85</td>
<td>2422.27</td>
</tr>
<tr>
<td>Test: CoV</td>
<td>0.028</td>
<td>0.008</td>
<td>0.010</td>
<td>0.064</td>
</tr>
<tr>
<td>DEM Simulation (Kg/m³)</td>
<td>2085.02</td>
<td>2237.25</td>
<td>2357.11</td>
<td>2447.89</td>
</tr>
<tr>
<td>% Difference</td>
<td>-7.4%</td>
<td>-3.7%</td>
<td>-1.8%</td>
<td>1.1%</td>
</tr>
</tbody>
</table>

**Figure 9 - Experiment-DEM comparison of flow function**

**Figure 10 - Stress-strain response comparison**
The experimental data shows a clearly defined peak and subsequent drop off in unconfined strength for the iron ore fines that is typical for a material that has been previously over-consolidated (Figure 10). However, the DEM simulations fail to capture this over-consolidation behaviour and instead display a more ductile response, where the peak strength is achieved and maintained for a prolonged strain. Further research is being conducted to investigate this mismatch.

6 CONCLUSIONS

This paper presented a summary of an adhesive elasto-plastic contact model that has been implemented in the commercial DEM code EDEM. Using this new contact model, DEM simulations have been carried out to simulate uniaxial tests on iron ore fines at a moisture content of 2%.

The numerical results have shown that it is possible to simulate the unconfined strength that is dependent on the consolidation stress, which is evident in the experimental data, and hence, to a certain degree match the flow function for iron ore fines. While an exact match to the experimental data has not been achieved yet in terms of the unconfined stress-strain response for iron ore fines, it was found that a reasonable match to the experimental flow function could be achieved. It is also possible to achieve a closer match to the experimental flow function but at the sacrifice of matching the confined consolidation behaviour of the iron ore fines. A parametric investigation is underway to build up a comprehensive understanding of influence of the DEM parameters on predicted bulk behaviour, including introducing a more realistic power law force-displacement relationship. This will underpin the work to derive a robust relationship between the bulk material properties and the contact model parameters.

7 ACKNOWLEDGEMENTS

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QUALITATIVE STATISTICAL ANALYSIS OF SIMULATED DATA FROM A PILOT SCALE MILL

JOHANNA ALATALO*, † AND BERTIL I. PÅLSSON†

* Research & Development
LKAB
SE-971 28 Luleå, Sweden
e-mail: johanna.alatalo@lkab.com, www.lkab.com

† Division of Sustainable Process Engineering
Luleå University of Technology
SE-971 87 Luleå, Sweden
e-mail: johanna.alatalo@ltu.se, www.ltu.se

e-mail: bertil.palsson@ltu.se, www.ltu.se

Key words: Comminution, tumbling mills, DEM, statistical analysis

Abstract. Grinding is the process of reducing a particle size distribution of an extracted ore and is commonly performed in a tumbling mill. It is a complex procedure and there is a lack of knowledge of what really happens inside the mill.

A number of pilot-scale experiments were done at LKAB's pilot plant at Malmberget, Sweden [1]. In this particular pilot mill, a continuous charge measurement system is installed in one of the lifters and it gives a deflection signal produced by the mill charge. From this signal it is possible to detect features correlated to the settings of the mill. Large, real experiments are very difficult to control and are of course, very costly and time consuming.

A 10 cm slice of the mill was simulated with discrete element method (DEM) for different mill operating conditions. From the simulations a deflection signal was extracted and validated against real data. There is a difference in the signal, mainly due to the lack of slurry in the simulations, but the behaviour when the mills operating conditions changes seems to be the same in both the simulated and the measured signals.

To analyse the data from the simulation a statistical analysis on a full factorial design was done. Two levels of degree of filling of the mill, two different rotational speeds, two levels of friction and different types of particles were selected as factors. The response data are two angles: toe and shoulder angle. The toe angle is when the lifter hits the charge and the shoulder angle is when the lifter leaves the charge.

The analysis show that the toe angle increases when the degree of filling is low and the rotational speed is high. It is also clear that the particle shape influences the charge behaviour. The simulated changes correspond to changes detected in pilot mill runs. This is important since it validates the DEM model.

In essence, mill simulations are easily done and the changes of factor levels cause the simulated mill to react in similar manner as in real cases. One advantage is that in simulations
one factor can be isolated and changed while the others are kept at constant values, which in turn creates the possibility to investigate one factor at a time. In real experiments, the factors are more dependent on each other and there is a very high disturbance from noise.

1 INTRODUCTION

In the North of Sweden, LKAB (Loussavaara Kirunaavaara AB) mines iron ore and produces upgraded iron ore products for the steel industry. To provide this, the particle size distribution of the extracted ore (mainly magnetite) needs to be decreased and this is done by grinding in tumbling mills in the concentrating plant. Comminution is a complex procedure; but still, it is necessary that the final product from the concentrator meet the required targets for iron content and the specified amount of fine material < 45 µm.

The product from the tumbling mill depends on size fraction of the feed material, the quality and the mineralogy of the ore. It is normally controlled by charge type, rotational speed of the mill, degree of filling inside the mill and the feed rate to the mill. The charge type can be the ore itself – so called autogenous grinding, pebbles – a selected size fraction of the ore or gangue, or manufactured media, usually steel rods or spheres (balls). However, it is difficult to control the product since the natural variation of the ore means that there is a varying optimal setting for the mill.

To be able to have control of the product, it is important to understand the grinding process. This is best done by experimental work, however they are not only difficult to control but also both costly and time consuming and therefore the number of experiments will necessarily be limited. Simulations are easily done of the mill and many different settings for the mill can be tested. This means that simulations offer a great possibility to increase the knowledge of what actually is occurring inside the mill. However, it is crucial that the simulations are verified against real process data to be trusted.

In order to get process data, experimental work has to be done and it is also necessary to have results to compare the simulations with. LKAB did experiments with a steel ball charge at their pilot plant in Malmberget, Sweden [1], and the same mill has also been used for experiments with a magnetite pebbles charge [2]. The pilot mill has an in-mill sensor installed that measures the deflection of a lifter. It is a continuous charge measurement (CCM) system provided by Metso Minerals. The sensor systems register the deflection of the lifter caused by the mill charge load on the lifter. From the signal it is possible to detect features that may be correlated to the settings of the mill. This curve can also be used to verify the experienced force on a simulated lifter. It is important to note, that the aim of the simulations are not to match the deflection curves to real experiments, since only the grinding media and no slurry or feed material is simulated, but to see if the response to changes is the same for both simulations and experiments. Thereby, verifying the simulations and also being able to investigate how other changes of variables effect the deflection of the lifter.
2 VERIFICATION OF SIMULATIONS WITH EXPERIMENTAL RESULTS

Experiments were done at LKAB and the results have been used to verify simulations. The first set of experiments with a steel charge show that there is a difference in the deflection, especially in the toe angle. Again, one major difference to the real experiments is the presence of slurry in the mill. The results show that the toe angle is lower and that the width of the deflection signal is not the same. The smaller width means that the charge is more compact in the simulations. It has been shown that three dimensional simulations are preferable over simulations in two dimensions. [3]

Comparison of deflection curves from experiments with a magnetite pebbles charge also has a discrepancy in the toe angle and width, consistent with the previous results with a steel charge. However, the simulations pick up the behavioural changes, such as an increased width when the degree of filling in the mill is increased.

Figure 1: A simplified view of the mill with toe and shoulder angles and the resulting deflection curve of one revolution. The height of the signal corresponds to the amount of deflection as the lifter passes through the charge.
Figure 2: Comparison of deflection curves of the simulated magnetite pebbles and experimental results.

The simulation results can not be used for predicting product results from the mill yet, but can at least be used to increase the knowledge of the events inside mill

3 SIMULATIONS

A 10 cm slice of the pilot mill with periodic boundaries was simulated with discrete element method (DEM) for different mill operating conditions. A full factorial test were done with two level of degree of filling, two different rotational speeds, two levels of friction, two different densities and two different shapes of the charge media; spheres or ellipsoids. The shape of the charge media is chosen to replicate the steel ball charge from the first set of experiments and the magnetite pebbles from the second set of experiments. The responses are the toe and shoulder angle in degrees. The test set-up can be seen in table 1. The simulations were done in a randomized order.

Table 1: The test set-up with factor levels

<table>
<thead>
<tr>
<th>Factor</th>
<th>Low</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Degree of filling</td>
<td>25 %</td>
<td>45 %</td>
</tr>
<tr>
<td>B % of critical speed</td>
<td>73 %</td>
<td>78 %</td>
</tr>
<tr>
<td>C Friction</td>
<td>0.5</td>
<td>0.8</td>
</tr>
<tr>
<td>D Density</td>
<td>5200 kg/m³</td>
<td>7800 kg/m³</td>
</tr>
<tr>
<td>E Shape</td>
<td>Sphere</td>
<td>Ellipsoid</td>
</tr>
</tbody>
</table>
The low and high level, 25 and 45 %, of degree of filling are common levels in conventional milling. The rotational speed are given as percentage of critical speed, the lowest speed possible to make a particle stick to the mill wall throughout the whole revolution, and the chosen speeds were used for the first the set of experimental work. The low and high levels of friction are chosen for steel on steel (0.8) and a lower value (0.5) to simulate a more slippery charge. The low and high value for the density is chosen to resemble the density of magnetite pebbles and steel balls, respectively. The shape is also chosen to resemble the steel balls and magnetite pebbles.

The three-dimensional simulations done are performed in EDEM [4] developed by DEM Solutions Ltd. The simulations have run for a number of revolutions and then averaged to decrease the influence of noise. A 20 second simulation of the mill takes approximately 8 hours to run.

![Figure 3: A simulated slice of the mill, where the individual particles are coloured by its absolute speed.](image)

4 RESULTS AND DISCUSSIONS

Toe and shoulder angles have been collected from each simulation, see table 2, and analysed with the aid of a statistical programme, Modde by Umetrics AB [5].
Table 2: Factorial levels and resulting responses from the simulations.

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>Toe angle</th>
<th>Shoulder angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
<td>Low</td>
<td>Low</td>
<td>Low</td>
<td>High</td>
<td>60</td>
<td>192</td>
</tr>
<tr>
<td>Low</td>
<td>Low</td>
<td>High</td>
<td>Low</td>
<td>Low</td>
<td>52</td>
<td>199</td>
</tr>
<tr>
<td>Low</td>
<td>Low</td>
<td>Low</td>
<td>High</td>
<td>Low</td>
<td>55</td>
<td>205</td>
</tr>
<tr>
<td>Low</td>
<td>Low</td>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>60</td>
<td>193</td>
</tr>
<tr>
<td>Low</td>
<td>High</td>
<td>Low</td>
<td>Low</td>
<td>Low</td>
<td>54</td>
<td>197</td>
</tr>
<tr>
<td>Low</td>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>High</td>
<td>64</td>
<td>193</td>
</tr>
<tr>
<td>Low</td>
<td>High</td>
<td>Low</td>
<td>High</td>
<td>High</td>
<td>63</td>
<td>211</td>
</tr>
<tr>
<td>Low</td>
<td>High</td>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>55</td>
<td>195</td>
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<tr>
<td>High</td>
<td>Low</td>
<td>Low</td>
<td>Low</td>
<td>High</td>
<td>42</td>
<td>201</td>
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<tr>
<td>High</td>
<td>Low</td>
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<td>Low</td>
<td>High</td>
<td>53</td>
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<tr>
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<td>Low</td>
<td>Low</td>
<td>High</td>
<td>High</td>
<td>56</td>
<td>206</td>
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<tr>
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<td>Low</td>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>41</td>
<td>205</td>
</tr>
<tr>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>Low</td>
<td>High</td>
<td>59</td>
<td>200</td>
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<tr>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>Low</td>
<td>Low</td>
<td>44</td>
<td>209</td>
</tr>
<tr>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>High</td>
<td>Low</td>
<td>46</td>
<td>211</td>
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<tr>
<td>High</td>
<td>High</td>
<td>High</td>
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<td>Low</td>
<td>49</td>
<td>206</td>
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<tr>
<td>Low</td>
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<td>198</td>
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<tr>
<td>Low</td>
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<td>208</td>
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<td>Low</td>
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<tr>
<td>Low</td>
<td>Low</td>
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<td>High</td>
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<td>61</td>
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<tr>
<td>Low</td>
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<td>Low</td>
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<tr>
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<td>47</td>
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<tr>
<td>High</td>
<td>Low</td>
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<td>Low</td>
<td>59</td>
<td>200</td>
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<tr>
<td>High</td>
<td>Low</td>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>57</td>
<td>201</td>
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<tr>
<td>High</td>
<td>Low</td>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>43</td>
<td>214</td>
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<tr>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>High</td>
<td>Low</td>
<td>59</td>
<td>203</td>
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<tr>
<td>High</td>
<td>Low</td>
<td>Low</td>
<td>Low</td>
<td>High</td>
<td>46</td>
<td>213</td>
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<tr>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>High</td>
<td>Low</td>
<td>45</td>
<td>214</td>
</tr>
<tr>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>High</td>
<td>High</td>
<td>58</td>
<td>212</td>
</tr>
</tbody>
</table>
The analysis shows that the toe angle is influenced by degree of filling, the rotational speed and the shape of the particles. There is also a slight interaction effect from degree of filling and the shape of particles, where the toe angle is affected more for a change in degree of filling when the particles are spherical than for ellipsoidal particles.

The main effects on the toe angles can be seen in figure 4. An increase in degree of filling causes the toe angle to decrease, which is anticipated since there simply is more material inside the mill. An increase in rotational speed will cause an increase in toe angle. An ellipsoidal shape will give a large increase for the toe angle compared to a spherical shape. This is a very interesting result since it means that the shape of the particle influence the movements of the charge.

**Figure 4:** The main effect on the toe angle by the degree of filling, the rotational speed and the shape of particles. N is the number of experimental runs, DF is the degree of freedom of the residuals, R2 – percent of variation of the response explained by the model, Q2 – the percent of the response predicted by the model according to cross validation, R2 Adj – R2 adjusted for degrees of freedom, RSD – residual standard deviation and Conf. lev. – confidence level.

The main effect on the shoulder angle is the degree of filling, the density and the shape of the particles, which can be seen in figure 5. An increase in degree of filling will cause an increase in shoulder angle, which is anticipated due to more material in the mill. An increase in the density causes an increase in shoulder angle. An ellipsoidal shape will give a smaller shoulder angle.
A high rotational speed will give a higher toe angle, this means that the charge has climbed higher in the mill and this result also correspond to the real deflection curves from the mill.

A high degree of filling gives a lower toe angle and a higher shoulder angle, this is anticipated since there simply is more material inside the mill and it corresponds very well with experimental results.

A high density will give a larger shoulder angle and this might be because the effect of each particle on the lifter is larger and is detected for a longer time.

A charge consisting of ellipsoidal particles will have a higher toe angle and a lower shoulder angle, this indicates a more compact charge than for the spheres. This is a very interesting result since it means that the shape of the particles is important for the dynamics in the charge.

5 CONCLUSIONS

The analysis show that the changes in toe angle correspond to changes detected in pilot mill runs. This is very important, since this also is a validation of the DEM model. It is also an indication that the material properties are important to get correctly.

In essence, mill simulations are easily performed and not nearly as time or cost consuming as real experiments. There is clearly an advantage to be able to perform simulation to
investigate operational changes for a mill. In a real experiment it is very difficult, if not impossible, to change the level of only one variable to detect the changes in the response, since the factors are more dependent on each other and there is a very high disturbance from experimental noise. This can be done in the simulations, where one parameter can be changed meanwhile the others are kept constant.

REFERENCES


RANDOM-WALK SIMULATION OF CELL MIGRATION AND PROLIFERATION

N. GARIJO¹*, R. MANZANO²ᵃ, R. OSTA²ᵇ AND M. A. PÉREZ¹ᵃ

¹: Multiscale in Mechanical and Biological Engineering (M2BE)
Aragón Institute of Engineering Research (I3A), University of Zaragoza,
Campus Río Ebro, c/María de Luna s/n, 50018-Zaragoza, Spain
e-mail: ³ngarijo@unizar.es; ³angeles@unizar.es

²: LAGENBIO-I3A, Instituto Aragonés de Ciencias de la Salud (IACS), University of Zaragoza
C/ Miguel Servet 177, 50013 Zaragoza, Spain
e-mail: ³rmanzano@unizar.es; ³osta@unizar.es

Key words: Migration, proliferation, stochastic (random-walk), adult muscle satellite cells

Abstract. Cell migration and proliferation has been modelled in several works of the literature as a process similar to diffusion. However, diffusion models to simulate the proliferation and migration of cells tend to create a homogeneous distribution in the cell density, but this result is not real. Diffusion is not the mechanism of cell dispersal: cells disperse by crawling or proliferation, or are transported in a moving fluid. The use of stochastic models or other (cellular automata, models particles, etc...) can modify this limitation. Therefore, this paper presents a stochastic model (random-walk) to simulate the proliferation and migration of cells. Both processes are considered as completely stochastic as discrete. The model developed aims to predict the behavior of in vitro cell cultures performed with adult muscle satellite cells. Non homogeneous distribution of cells has been observed inside the culture well. Using previous stochastic model we have been able to predict the non homogeneous cell distribution and accurate quantitative results have been computed. In a future, the model will allow us to incorporate other aspects such as cell differentiation, incorporate several cell populations simultaneously, etc.
1 INTRODUCTION

Cell migration and proliferation has been modelled in several works of the literature as a process similar to diffusion\cite{1}. Bailon-Plaza and van der Meulen (2003)\cite{2} simulate cell migration as a diffusive process taking account gradients in matrix density (haptotaxis). However, using a diffusion model to simulate the migration and proliferation tends to create a smooth variation in cell density, but this result may not be enough. The use of stochastic models (random-walk) or other (cellular automata, particles models, etc...) \cite{3,4} can modify this limitation. Furthermore, random-walk models can simulate not only a preferred direction of migration (resulting from, for e.g., convection or chemoattractant control of migration) but proliferation can also be explicitly modelled by multiplying cell numbers during dispersal. Moreover, using a random-walk model these aspects could be included for several cell populations simultaneously.

Experiments demonstrating random movement of cells were done many years ago. For example, Ambrose (1961)\cite{5} observed the movement of an isolated fibroblast over the surface of a tissue culture dish as mostly random while Carter (1965)\cite{6} was among the first to demonstrate that cells execute a random walk on surfaces. Gail and Boone (1970)\cite{7} quantified that cell migration differs from the pure random walk in that the angles between successive turns are closer to zero; therefore, cells show persistence in their movements. More recently, Palsson and Bahatia (2004)\cite{8} observed, in an in vivo analysis, that a random spatial distribution could be produced during stem cell proliferation. Zohar et al (1998)\cite{9} observed experimentally that mesenchymal stem cells (MSCs) disperse by crawling and convection in the fluid. The directional nature of movement is most apparent with fibroblasts; during wound healing, they become highly motile and migrate in large numbers towards the wound\cite{10}; diffusion-type models that reproduce this effect have been developed\cite{11,12}.

Therefore, this paper presents a stochastic model (random-walk) to simulate the proliferation and migration of cells\cite{13}. Both processes have been considered as completely stochastic. The model developed aims to predict the behavior of in vitro cell cultures performed with adult muscle satellite cells. Non uniform cells distribution has been observed inside the culture well\cite{14}. Satellite cells are stem cells or muscle pre-cells which serve to aid the regeneration of adult skeletal muscle\cite{15}. As result of the proliferation (when the cells are reproduced for satellite) and the latter differentiation (when the nucleus changes into a specific type of cell, in this case, a muscle cell), satellite cells are fused between them or with damaged muscle adjacent fibres, this increases the number of myonuclei in the fibres for its growth and regeneration. The proliferation of satellite cells is necessary for supplying more nuclei to the muscle cells. The differentiation is also necessary for the new nuclei to behave as muscular nuclei. The number of myonuclei directly determines the capacity of the muscle cell to produce proteins, including androgen receptor.

For the validation of the model several experiments have been performed with muscle satellite cells of control mouse Wild Type (WT) and transgenic (TR), moreover the cells come from two types of fibres - Fast (anaerobic) and aerobic – Slow (aerobic). The Fast cell type come from a tissue with a fast muscle contraction, while Slow cells type derive from tissue with postural functions\cite{16,17}.
2 MATERIAL AND METHODS

2.1 Cell proliferation

The approach for modelling the proliferation of cells is based on the random-walk theory. It is a stochastic process. Initially a cell is presumed (in two dimensions) to be surrounded by four locations that a daughter cell could occupy (Figure 1). Daughter cells are also allowed to remain in the position of the parent cell but opposite “poles” are excluded (as shown in Figure 1) because adjacent positions are far more likely to occur during mitosis. The cells can occupy neighbouring positions with equal probability \( p \) (see Figure 1). Although Figure 1 shows four free positions around the cell, this will not, in general, be the case because some positions may already be occupied. Therefore, the model incorporates “contact inhibition” by checking for vacant positions while cells proliferate and depending on the available states \( (n) \), the value of the probability \( p \) is computed in order to fulfil the condition \( \sum_{i=1}^{n} p_i = 1 \). If all the surrounded positions are free, the probability \( p \) given in Figure 1 will be equal to 1/4. If there is only one vacant position, the probability that it will be filled is equal to one. If all neighbouring positions are occupied, mitosis will not occur.

2.2. Cell migration \((n_s, t_s)\)

Cell migration was also based on the stochastic random-walk approach. Recognising that migration is a more rapid process, a new location for a migrating cell is chosen several times during one iteration of the proliferation process. In the stochastic model proposed, migration is controlled by two parameters: \( n_s \) the number of jumps that a cell performed during each proliferation iteration; and \( t_s \) the jump size, ie, the distance that the cell moves in each jump. In the simulations presented here, five random jumps are performed for each cell during each iteration of the simulation \((n_s=5\text{ and } t_s=1)\). The possible states that cell can occupy after migration, are defined by the nearest wall of the culture wells. At the end of the migration if that position is free is checked. In the event that the location has already been occupied by another cell, a neighbouring location is chosen again randomly, except if the cell population is large enough to prevent the migration of cells. In that case, cells remain in their initial position without migration (“contact inhibition”).

2.3 Cell migration \((n_s, t_s)\)

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chosen again randomly, except if the cell population is large enough to prevent the migration of cells. In that case, cells remain in their initial position without migration (“contact inhibition”).

![Figure 1: Different possible states for each cell that can occupy after the proliferation. The distance between the sites is only schematic; adjacent sites in the algorithm are considered to be exactly the diameter of a cell. [18].](image)

### 2.4 Experimental data

In vitro cell cultures with adult muscle satellite cells have been used to validate the model. In vitro cultures have been done in wells of 6.34 mm of diameter (plates of 96 wells) where 1000 cells were initially seeded in culture medium, which was changed daily. The experiment lasted for 5 days during which markers indicating proliferation or mitosis, and differentiation were measured. There were mainly 4 types of experiments depending on the mouse type and the muscle type where that the cells were extracted. There were two mouse types: wild type (WT) and transgenic mouse (TR) which is used as a neurodegenerative model. Cells were extracted from two different muscle tissues: Fast (Anaerobic fibres) when the cells came from a tissue with a fast muscle contraction and Slow (Aerobic fibres) when they came from a tissue with postural functions. For each type of experiment, cells were daily counted and 8 repetitions of each test were done. In each well, cells were counted in 4 areas that correspond to the lateral sides. Therefore, from each well there were 4 data, and a total of 32 values. Mean values were computed and from them, the proliferation rate in each case was obtained. A summary of the experimental data (rate of proliferation) is shown in the Table 1.

<table>
<thead>
<tr>
<th>Mouse</th>
<th>Fibre type</th>
<th>Day 0</th>
<th>Day 1</th>
<th>Day 2</th>
<th>Day 3</th>
<th>Day 4</th>
<th>Day 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>WT</td>
<td>Fast</td>
<td>0.00</td>
<td>2.52</td>
<td>2.14</td>
<td>3.99</td>
<td>2.15</td>
<td>1.94</td>
</tr>
<tr>
<td>TR</td>
<td>Fast</td>
<td>0.00</td>
<td>2.38</td>
<td>2.56</td>
<td>2.35</td>
<td>2.07</td>
<td>1.80</td>
</tr>
<tr>
<td>WT</td>
<td>Slow</td>
<td>0.00</td>
<td>1.29</td>
<td>1.88</td>
<td>3.54</td>
<td>2.14</td>
<td>1.26</td>
</tr>
<tr>
<td>TR</td>
<td>Slow</td>
<td>0.00</td>
<td>2.02</td>
<td>1.47</td>
<td>2.58</td>
<td>2.18</td>
<td>1.72</td>
</tr>
</tbody>
</table>

**Table 1:** Summary of the proliferation rate in cell culture in vitro.
It was observed that the proliferation behavior was different depending on the mouse type and the muscle fibres from which the cells were extracted. Fast cells proliferated more than from Slow ones. There were also differences between the mouse types (WT vs. TR), the proliferation rate was lower in transgenic mice (TR) and its proliferation rates were also more uniform during the whole experiment.

2.5 Implementation algorithm

The algorithm implementation has been represented in the Figure 2. The simulation starts with an initial population of 1000 cells (as in the experiments) randomly distributed in the cell culture. The cells begin to proliferate following the process indicated in section 2.1. The proliferation rate indicates the percentage of population that will proliferate. If the ratio is 100%, all cells proliferate, but if the ratio is lower, the cells that proliferate are selected randomly between the population. It have been defined two parameters that control the proliferation rate: \( p_1 \) controls the mouse type (Wild Type WT or transgenic TR); \( p_2 \), defines the proliferation rate depending on the fibres type (Fast or Slow). The combination of both parameters results in the proliferation rate \( p_r = p_1.p_2 \). The values considered for these parameters have been shown in Table 2. The algorithm also allows to consider preferential directions of the proliferation. The cells prefer to take location near the wells edges.

Once the cells have proliferated, migration is simulated using the random-walk theory described in Section 2.2. The migration process is controlled by two parameters: the number of jumps \( (n_s) \) and the jump size \( (t_s) \). The values used in the simulation have been shown in Table 2.
Table 2: Parameters of the model used in this simulation.

<table>
<thead>
<tr>
<th></th>
<th>p1 (%)</th>
<th>p2 (%)</th>
<th>Migration</th>
</tr>
</thead>
<tbody>
<tr>
<td>WT</td>
<td>100</td>
<td>Fast</td>
<td>100</td>
</tr>
<tr>
<td>TR</td>
<td>80</td>
<td>Slow</td>
<td>65</td>
</tr>
</tbody>
</table>

After migration, if the new random position is occupied is checked (check the collision - Figure 2). If the position is occupied, one of the cells is removed (apoptosis) and the number of collisions equals the number of cells removed. This process is known in biology as contact inhibition. Finally, the new population initiates a new cycle (Figure 2).

3. RESULT

The proliferation rate obtained from the simulation for the different cases considered and their comparison with the experimental results obtained during 5 days of cell culturing have been represented in Table 3. To obtain the computational results, 5 simulations of each case have been performed. As the simulation is based on a stochastic model, it provides a different result each time. Therefore, the average values of the results have been calculated. The results have been shown in Table 3.

Table 3: Summary of the proliferation rates from experimental test and computational simulations.

<table>
<thead>
<tr>
<th>Mouse</th>
<th>Fibres type</th>
<th>Day 1</th>
<th>Day 2</th>
<th>Day 3</th>
<th>Day 4</th>
<th>Day 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>WT</td>
<td>Fast</td>
<td>Experimental 2.52</td>
<td>2.14</td>
<td>3.99</td>
<td>2.15</td>
<td>1.94</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Computational 2.60</td>
<td>2.31</td>
<td>4.53</td>
<td>2.61</td>
<td>1.78</td>
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<tr>
<td>TR</td>
<td>Fast</td>
<td>Experimental 2.38</td>
<td>2.56</td>
<td>2.35</td>
<td>2.07</td>
<td>1.80</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Computational 2.22</td>
<td>2.02</td>
<td>3.57</td>
<td>2.38</td>
<td>1.83</td>
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<tr>
<td>WT</td>
<td>Slow</td>
<td>Experimental 1.29</td>
<td>1.88</td>
<td>3.54</td>
<td>2.14</td>
<td>1.26</td>
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<tr>
<td></td>
<td></td>
<td>Computational 1.97</td>
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<td>3.07</td>
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<tr>
<td>TR</td>
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<td>2.58</td>
<td>2.18</td>
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<tr>
<td></td>
<td></td>
<td>Computational 1.69</td>
<td>1.61</td>
<td>2.42</td>
<td>1.98</td>
<td>1.75</td>
</tr>
</tbody>
</table>

It can be observed in Table 3, as the proliferation rates are very similar between computational and experimental results. The differences may be due to that the differentiation process has not been incorporated in the simulation yet. Special markers were added in the in vitro cultures to indicate if there is cell differentiation. In fact their values indicated that cells experienced differentiation, therefore these differentiated cells stop proliferating. This fact could explain the small differences in the proliferation rates.

During the first days of the experiments, it was observed that cells were not homogeneously distributed across the surface of the well, but it had a greater cell density in the lateral than in the center (Figure 3a). In the simulation, something similar was predicted, especially during the first three days. There is more concentration of satellite cells in the lateral region of the well than in its center (Figure 3b). By continuing the simulation it can be appreciate that as the number of cells increase, they are distributed uniformly in the culture well.
The results shown in Figure 3b, were obtained using 5 jumps (ns) during migration and the jump size is 1 (ts). We performed a sensitivity study of these parameters (see Figure 4). It can be observed as increasing the number of jumps (ns) (Figure 4a and b), the cellular distribution is more uniform and there are more cells quantitatively distributed than with a lower number of jumps (Figure 3b). Something similar happens with the size (ts), ie, the distance traveled by the cell at each jump. By increasing the size (Figure 4c and d) a more homogeneous distribution of cells in the culture well is predicted.

4 DISCUSSION

The methodology presented in this paper proposes the use of a stochastic model of random walk to simulate the behaviour of muscle satellite cells, both proliferation and migration [13]. The computational results are similar to those obtained in in-vitro cultures [14] both qualitatively and quantitatively. The proliferation rates between the two results are similar, with slight differences that come from the fact that the simulations do not incorporate differentiation, and experimentally it was demonstrated that there was differentiation by the presence of markers since the third day (Table 3). The proposed methodology has been qualitatively validated by observing the cell population distribution that the different studies of the literature had described, which confirm the random mobility of muscle satellite cells, although no quantitative results have been described. Hence a sensitivity analysis has been done to determine the influence of the migration parameters. It has been reported that they fundamentally affect the homogeneity in the distribution of cells in the culture well. Another limitation of the model is that cell differentiation has not been incorporated, but it will be incorporate in a future work.
In conclusion, the stochastic model of random walk presented in this paper is an approach that simulates cell proliferation and migration, with a methodology that can be easily implemented to simulate problems related to biologic mechanisms or tissue engineering.

![Figure 4: Cell distribution in the well after 5 day simulation compared with parameters different of migration \((n_s, t_s)\): (a) \(n_s=7, t_s=1\); (b) \(n_s=10, t_s=1\); (c) \(n_s=5, t_s=3\); (d) \(n_s=7, t_s=3\).]

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NUMERICAL SIMULATIONS OF SAND BEHAVIOUR USING DEM WITH TWO DIFFERENT DESCRIPTIONS OF GRAIN ROUGHNESS

J. KOZICKI AND J. TEJCHMAN

Civil and Environmental Engineering Department
Gdańsk University of Technology
Gdańsk, Poland

e-mail: jkozicki@pg.gda.pl, tejchmk@pg.gda.pl

Key words: DEM, Dissipation, Energy, Grain Roughness, Sand, Triaxial Test

Abstract. A quasi-static homogeneous drained triaxial compression test on cohesionless sand under constant lateral pressure was simulated using a three-dimensional DEM model. Grain roughness was modelled by two different approaches: first with contact moments applied to rigid spheres and second with clusters of rigid spheres imitating irregular particle shapes. The effect of the grain roughness (shape) on shear strength, dilatancy, energy and dissipation was analyzed using both models. Numerical results were directly compared with experimental results on Karlsruhe sand.

1 INTRODUCTION

Granular materials consist of grains in contact and of surrounding voids, which change their arrangement depending on environmental factors and initial density. Their micromechanical and fabric behaviour is inherently discontinuous, heterogeneous and non-linear. To describe their behaviour, two main approaches are used: continuum and discrete ones. The first ones perform simulations at the global scale using the finite element method on the basis of e.g. elasto-plastic and hypoplastic constitutive models enhanced by a characteristic length of micro-structure to describe strain localization. In turn, the latter ones perform simulations at the grain scale, i.e. each grain is modelled individually. Their advantages are that they directly model micro-structure and can be used to comprehensively study the mechanism of the initiation, growth and formation of shear zones at the micro-level which strongly affect macro-properties of granular matter. The disadvantages are: high computational cost, inability to model grain shape accurately, difficulty to validate it experimentally and inertial effects and damping effects lose their meaning in quasi-static problems. However, they become more and more popular nowadays for modelling granular materials due to an increasing speed of computers and a connection possibility to the finite element method.

Many experimental and numerical studies revealed that irregularly shaped grains strongly affect the quasi-static mechanical behavior of granular materials. To resemble the real grain shape (roughness), two main approaches are usually used: 1) contact moments between rigid spheres or disks [1-6]) or clusters of combined discrete elements that form irregularly-shaped grains [7-11].

In this paper, numerical studies of quasi-static homogeneous axisymmetric triaxial compression tests were carried out to determine the macroscopic behaviour of a sand...
specimen composed of discrete elements. The three-dimensional discrete model YADE developed at University of Grenoble was used [3]. The particle breakage has not been considered. Discrete simulation results were quantitatively compared with the corresponding experimental data from drained axisymmetric triaxial compression tests performed by Wu [12] at Karlsruhe University with real sand. The intention of our studies was to calculate the effect of the grain roughness (shape) using these two above mentioned methods on the shear strength, dilatancy, energy and dissipation of real sand (so-called Karlsruhe sand), which had the same initial void ratio, mean grain diameter and grain distribution. Such a direct comparison of the effect of grain roughness using 2 different approaches has not been performed yet. A special attention was paid to the energy transformation in sand and its elastic and dissipative characteristics, playing an important role in the granular matter behaviour. The energy and dissipation results were compared with the similar ones during two-dimensional simulations of biaxial compression with round particles performed by Kruyt and Rothenburg [13] and by Bi et al. [14].

2 DISCRETE ELEMENT METHOD

The discrete element method (DEM) is widely used to model a range of processes across many industries. To simulate the behaviour of sand, a three-dimensional spherical discrete model YADE was developed at University of Grenoble [3] by taking advantage of the so-called soft-particle approach (i.e. the model allows for particle deformation which is modeled as an overlap of particles). A dynamic behaviour of the discrete system is solved numerically using a force-displacement Lagrangian approach and tracks the positions, velocities, and accelerations of each particle individually. It uses an explicit finite difference algorithm assuming that velocities and accelerations are constant in each time step. To calculate forces acting in particle-particle or particle-wall contacts, a particle interaction model is assumed in which the forces are typically subdivided into normal and tangential components. The total forces acting on each particle are summed. Next, the problem is reduced to the integration of Newton’s equations of motion for both translational and rotational degrees of freedom. As the results, the accelerations of each particle are obtained. The time step is incremented and accelerations are integrated over time to determine updated particle velocities and positions. To maintain the numerical stability of the method and to obtain a quick convergence to a quasi-static state of equilibrium of the assembly of particles, damping forces have to be introduced [15]. To increase the rolling resistance, contact moments between spheres (caused by the normal force) were introduced [3]. Figure 1 shows the mechanical response of contact models.

The following five main local material parameters are needed for discrete simulations: $E_c$ (modulus of elasticity of the grain contact), $\nu_c$ (Poisson’s ratio of the grain contact), $\mu$ (inter-particle friction angle), $\beta$ (rolling stiffness coefficient) and $\eta$ (plastic rolling coefficient) using spheres with contact moments ($E_c$, $\nu_c$ and $\mu$ without contact moments). In addition, the particle radius $R$, particle density $\rho$ and damping parameters $\alpha$ are required. The material parameters were calibrated with corresponding axisymmetric triaxial laboratory test results on Karlsruhe sand by Wu [12]. The index properties of Karlsruhe sand are: mean grain diameter $d_{50}=0.50$ mm, grain size among 0.08 mm and 1.8 mm, uniformity coefficient $U=2$, maximum specific weight $\gamma_d^{\text{max}}=17.4$ kN/m$^3$, minimum void ratio $e_{\text{min}}=0.53$, minimum specific weight $\gamma_d^{\text{min}}=14.6$ kN/m$^3$. 
and maximum void ratio $e_{\text{max}}=0.84$. The following discrete material parameters for rigid spheres with contact moments were assumed for discrete studies: $E_c=0.30$ GPa, $\nu=0.3$, $\mu=30^\circ$, $\eta=0.2$, $\beta=0.1$, $\rho=2.6$ kN$s^2$/m$^4$, $\alpha=0.08$ and $d_{50}=5.0$ mm.

![Diagram of contact models](image.png)

**Figure 1**: Mechanical response of contact models: a) tangential contact model, b) normal contact model and c) rolling contact model [3]

In numerical simulations, a cubic sand specimen of $10\times10\times10$ cm$^3$ was used. A simplified linear grain distribution curve was used for Karlsruhe sand (grain range among 2 mm and 8 mm). In order to save the computation time, remaining discrete simulations showing the capabilities of DEM were carried out with $d_{50}=5$ mm instead of $d_{50}=0.5$ mm. The test was modelled using confining smooth rigid wall elements (without inducing shear localization). The top and bottom boundaries moved vertically as loading platens under strain-controlled conditions to simulate the confining pressure $p$. To ensure the test was conducted under quasi-static conditions, the loading speed was slow enough. The initial configuration of the sand specimen was isotropic. Each assembly was prepared by first dropping the particles into the container under a gravitational field with the friction coefficient between particles set to zero. Gravity was varied to obtain a desired initial density caused by grain overlapping (thus, it was possible to exactly reproduce the experimental initial sand volumetric weight). The assembly was then allowed to settle to a state where the kinetic energy was negligible, before it is compressed under an initial confining pressure. The isotropic assembly was then subjected to boundary driven triaxial compression.
Figure 2 presents the 12 different clusters of spheres used in discrete calculations. In the case of the cluster of 2 spheres without the overlap (shape ‘f’), 26’300 clusters were used composed of 52’600 spheres. In turn, 28’250 clusters were used with 197’750 spheres to model simple ellipsoids (shape ‘i’) and 14’500 clusters were used with 594’500 spheres to model disks (shape ‘l’). In the case of 3D calculations with spheres using contact moments, 6’600 spheres were used.

3 DISCRETE RESULTS OF TRIAXIAL TEST

3.1 Effect of grain roughness (shape) on strength and volume changes

Figure 3 shows the calculated evolution of the vertical normal stress and overall void ratio versus vertical normal strain for different clusters of spheres of Fig.2 (without contact moments) during triaxial compression with initially dense sand ($e_0=0.53$, $d_{50}=5$ mm) under confining pressure of $p=200$ kPa. Similarly as in the real experiment (Fig.3), the initially dense specimens exhibits initially elasticity, hardening (connected to contractancy and dilatancy), reaches a peak at about of $\varepsilon_l=3\%$, gradually softens and dilates reaching at large vertical strain of 25-30% the same value of the vertical normal stress with the granular specimen deforming at constant volume, i.e. a critical state is always reached. Thus, the particle shape is not essential for the global critical internal friction angle (except of the case with spheres). The both mobilized strength and dilatancy increase with increasing grain roughness (rolling resistance) combined with an increase of the sphere number. Thus, the irregularly shaped particles provide obviously higher internal friction angles and have less tendency to rotate than perfect circular particles. The global maximum mobilized internal friction angle increases from $\phi_{\text{max}}=28^\circ$ (spheres) up to $\phi_{\text{max}}=48.9^\circ$ (disks), respectively (Fig.3). In turn, the global residual internal friction angle increases from $\phi_{\gamma}=15^\circ$ (spheres ‘a’ of Fig.2) up to $\phi_{\gamma}=31^\circ$ (disks ‘l’ of Fig.2), respectively (Fig.3). The dilatancy angle $\psi$ raises from $\psi=5^\circ$
(spheres) up to $\psi = 30^\circ$ (disks), respectively. The elastic modulus is also similar independently of the grain roughness. The granular system shows small fluctuations in the residual phase.

Figure 4 shows a direct comparison between different granular clusters composed of 2 ellipsoids, 2 spheres and 6 spheres without contact moments, pure spheres with contact moments and experiments (Wu 1992). All curves are qualitatively the same. The global maximum internal friction angle is $42.5^\circ$ at $\varepsilon_1 = 5\%$ (spheres with contact moments) and $41^\circ$ (clusters) $\varepsilon_1 = 3\%$. In turn, the global residual internal friction angle is $32.5^\circ$ (spheres with contact moments) and $31^\circ$ (clusters). As compared to the results with spheres with contact moments, the best agreement with experiments provides clusters of 6 spheres. Note that it is possible to calibrate more accurately a discrete model with each grain shape of Fig.2 with respect to laboratory tests.

3.2 Effect of grain roughness (shape) on energy and dissipation

In the granular system there exist 3 main energies: the elastic energy, kinetic energy and energy dissipation. In addition, numerical dissipation also exists. The elastic internal energy stored at contacts between grains $E_e$ is done by elastic contact tangential forces on tangential
elastic displacements $U$, contact normal forces on penetration depths $U$ and elastic contact moments on elastic rotations $\omega$ (when contact moments are considered). In general, the elastic internal energy is $(N - \text{contact number})$. The kinetic energy $E_k$ of grains is caused by their translation and rotation. Due to quasi-static conditions, the effect of $E_k$ is negligible (less than 1%). The energy plastic dissipation $D_p$ is due to plastic (shear) tangential forces and plastic (shear) moments during slip (sliding) and rotation (see Fig.1). In addition, numerical dissipation $D_n$ takes place during translation and rotation. The total accumulated energy $E = E_e + E_c + D_p + D_n$ is equal to the external boundary work $W$ done on the assembly by 6 external forces on displacements of 6 rigid external walls.

**FIGURE 4**: Effect of some clusters of spheres of Fig.2 without contact moments and single spheres with contact moments on vertical normal stress $\sigma_1$ versus vertical normal strain $\varepsilon_1$ (A) and volumetric strain $\varepsilon_v$ versus vertical normal strain $\varepsilon_1$ (B) compared to experiments (→) during homogeneous triaxial compression test ($e_s = 0.53$, $p = 200$ kPa, $d_{50} = 5.0$ mm)

Figure 5 shows the calculated effect of the grain roughness on the total accumulated energy $E$, elastic internally stored energy at contacts $E_e$, plastic dissipation $D_p$ and numerical damping $D_n$ (Eq.8) in initially dense sand ($e_s = 0.53$, $p = 200$ kPa, $d_{50} = 5.0$ mm). Compared were the systems composed of spheres with contacts moments and systems of clusters of 2 spheres and 6 spheres without contact moments (Fig.2). In turn, the evolution of the external energy rate $\delta E$, elastic internal energy rate $\delta E_e$ and plastic dissipation rate $\delta D_p$ is demonstrated in Fig.6. Finally, Figure 7 demonstrates the evolution of the kinetic energy of the systems.

There exists a roughly linear relationship between the total energy and plastic damping against the vertical normal strain (Fig.5). The plastic dissipation during frictional sliding is equal at the strain of $\varepsilon_1 = 3\%$ (corresponding to the maximum vertical stress) to 50% of the total energy (irregularly-shaped grains). At the residual state of $\varepsilon_1 = 30\%$, it is already equal to 88% (irregularly-shaped grains) of the total energy. The numerical damping is equal always to 6% of the total energy. The evolution of three components of the elastic internal energy is similar to the evolution of the shear strength (the maximum value is at $\varepsilon_1 = 5\%$) (Fig.3). At the beginning of deformation at $\varepsilon_1 < 1\%$ (when the specimen is in the elastic range), the total energy is almost fully converted into the elastic energy. The change of the elastic internal work is initially positive. It rapidly approaches zero and a small negative value at about $\varepsilon_1 = 5\%$ (Fig.6) and afterwards slightly increases approaching an asymptote at zero. Beyond
strains of $\varepsilon_i = 5\%$, almost the entire input work is dissipated due to plastic deformation and numerical damping (the external energy rate and dissipation rate are equal $\delta W = \delta D$).

Figure 5: Calculated evolution of: a) total energy $W$, b) plastic dissipation $D_p$, c) elastic work in normal direction $E_{el}^n$, d) elastic work in tangential direction $E_{el}^t$, e) numerical non-viscous damping $D_n$ during homogeneous triaxial compression test for: A) single spheres with contact moments, B) clusters of 2 spheres, C) clusters of 6 spheres ($\varepsilon_i = 0.53$, $p = 200$ kPa, $d_{50} = 5$ mm) (I) wide view, II) zoom)
Figure 6: Calculated evolution of: a) external energy rate $\delta W$, b) elastic internal work rate $\delta E_e$ and c) plastic energy dissipation rate $\delta D$ during homogeneous triaxial compression test: A) clusters of 2 spheres, B) clusters of 6 spheres ($e_0=0.53$, $p=200$ kPa, $d_{50}=5$ mm)

Figure 7: Calculated evolution of kinetic energy $E_k$ during homogeneous triaxial compression test: A) clusters of 2 spheres, B) clusters of 6 spheres ($e_0=0.53$, $p=200$ kPa, $d_{50}=5$ mm), a) translational kinetic energy, b) rotational kinetic energy

The elastic internal work is 80% at $\varepsilon_1=1\%$, 40% at $\varepsilon_1=3\%$ and 5% at $\varepsilon_1=30\%$ (irregularly-shaped grains) of the total energy, respectively. The residual elastic internal work is performed by contact normal forces in 70%, by contact tangential forces in 20% and by contact moments in 10% in the case of single spheres with contact moments, and by contact normal forces in 70% and contact tangential forces in 30% with irregularly-shaped grains. Thus, the largest internal work is performed by contact normal forces and the smallest one by contact moments. The elastic energy ratio is the same at the residual state.

The evolution curves in Figs.5 are qualitatively similar to those demonstrated by Bi et al. [14]. In turn, the evolution curves in Fig.6 are slightly different in the initial phase than those
shown by Kruyt and Rothenburg [13], which were calculated using periodic boundary conditions. The calculated energy quantities are different than in analyses by Bi et al. [14] using the software of PFC2D (where e.g. the calculated elastic energy was significantly higher: 90% (at $\varepsilon_1=3\%$) and 20% (at $\varepsilon_1=5\%$) of the total energy.

The kinetic energy is very small due to the quasi-static loading of the granular system (Fig.7). A release of the elastic energy drives grains to move. At the elastic stage, the rotational kinetic energy is close to zero. After it increases and slightly decreases. At the residual phase, the kinetic energy shows fluctuations which correspond to the evolution of the elastic energy and damping rate.

4 CONCLUSIONS

The numerical simulations of a homogeneous triaxial compression test show that a discrete model is capable to reproduce the most important macroscopic properties of cohesionless granular materials without it being necessary to describe the granular structure perfectly. Comparing the numerical simulations with the experimental triaxial tests conducted for different initial void ratios and confining pressures shows that the model is able to realistically predict the experimental results for cohesionless sand. The following detailed conclusions can be also drawn:

- The model is capable of closely reproducing the behaviour of cohesionless soils in the elastic, contraction, and dilatancy phase and at the critical state. At large strains, the granular specimen reaches always a critical state independently of its initial density. The higher the confining pressure, the smaller are both the global friction and dilatancy.
- The sand grain roughness can be modelled by means of spheres with contact moments or irregularly-shaped grains. The calculations with spheres are significantly faster, but those with irregularly-shaped grains are more realistic.
- The largest internal work is performed by contact normal force and the smallest one by contact moments.
- At the elastic stage, the boundary external work is mainly converted into elastic energy. At the residual state, the almost total external boundary work is dissipated by plastic deformation.
- The kinetic energy is very small due to quasi-static loading. The translational kinetic energy is higher than the rotational one.

Our research will be continued. The discrete simulations will be carried with sand during biaxial compression out by taking into account shear localization. The local phenomena occurring in a shear zone (such as buckling of granular columns, vortices, force chain cycles, periodic alternating dilatancy and contractancy) will be carefully studied.

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NUMERICAL STRESS PROBING ON A 2D MODEL GRANULAR MATERIAL

F. FROIIO*, J.-N. ROUX†

* Laboratoire de Tribologie et Dynamique des Systèmes
Ecole Centrale de Lyon, 36 av. Guy de Collongue
69134 Ecully cedex, France
e-mail: francesco.froiio@ec-lyon.fr, ltds.ec-lyon.fr

† Laboratoire Navier
Université Paris-Est, 2 Allée Kepler, Cité Descartes
77420 Champs-sur-Marne, France e-mail: jean-noel.roux@lcpc.fr, www.lcpc.fr

Key words: Granular Materials, DEM, Stress probing, Elastoplasticity

Abstract. We use DEM simulations on a simple 2D model of a granular material to measure its deformation response to small stress increments of arbitrary directions (stress probes) and assess the applicability of the classical concepts of elastoplasticity. We impose stress increments in the space of principal stresses components, to numerical specimens selected at various intermediate states along the biaxial compression path. The elastic part of the incremental response is systematically identified by building the elastic stiffness matrix of well-equilibrated configurations. Plastic strain increments are computed standing on the partition hypothesis for strain increments into elastic- and plastic parts. The domain of validity of the partition hypothesis is discussed, playing extensively with the magnitude of the stress increments, in order to identify a range in which the incremental response is homogeneous of degree 1 and the essential features of plasticity models can be observed. We investigate in particular the existence of a plastic flow rule with a clearly defined plastic flow direction and yield criterion. The robustness of these features is tested over a range of contact stiffness levels and against the dominant deformation modes (i.e., based on contact deformation or network rearrangement).

1 Introduction

Elastoplastic models for granular materials under quasistatic loading conditions were first developed by adapting the key features of metal plasticity models to the frictional-cohesive nature of soils, on a large basis of phenomenological observation in laboratory testing [1, 2]. The continuously improving performances of discrete numerical simulation tools offer nowadays the possibility to run reliable testing campaigns on “virtual” granular
specimens. In complement to physical testing, discrete numerical simulations provide flexibility, repeatability and an open window on the microscopic processes driving the phenomenologically observable behaviour. This paper summarizes some recent advances of an ongoing work that should be ascribed in the relatively small number of studies where the essential features of elastoplastic models for granular materials are investigated by a systematic use of a numerical implementation of the stress probing technique \[3, 4, 5\], as first addressed by Bardet \[6, 7\] since 1989. The simple idea of this technique is to measure the deformation response of “identical” specimens to a rose of supposedly-infinitesimal stress increments (stress probes) in a comprehensive spectrum of stress directions. Clearly, a prerequisite for this technique is the capability to obtain as many identical specimens as the number of stress increment directions under considerations. This facts makes its application prohibitive, therefore rare, in physical testing \[8\], while it entails no major difficulty in numerical testing.

Among the classical features of elastoplasticity that have been investigated by previous researchers applying the stress probing technique to granular materials, one can mention (i) the character of rate-independence of the material response, (ii) the partition hypothesis for the deformation increments into elastic- and plastic components and (iii) the existence of a plastic flow rule with clearly identified plastic flow direction and yield criterion. In this study, those features are reconsidered in an enlarged and unified context, by varying a small number of material- and texture parameters. In addition, we pay particular attention to (iv) the identification of an appropriate range of stress increment amplitudes for the measurements to be actually expressive of the incremental (tangent, infinitesimal) response. We show why this apparently technical aspect can affect the measurement results substantially. We limit ourselves, in this paper, to some results concerning stress probes under biaxial conditions. For some anticipations on the extension of the method to the incremental response under rotation of principal stress axes, we refer the interested reader to a preliminary study in Ref. \[9\].

In the following sections we introduce briefly the numerical procedure of specimen preparation and the inherent parameters. Next, we address some results concerning the issues at points (i)-(iv) in the above list and conclude with a short summary.

2 Specimen preparation and investigation points

The numerical samples tested in this work are disk assemblies of 5600 particles, with diameters uniformly distributed in the range $[0.7d, 1.3d]$ about the average diameter $d$. Two contacting particles interact by a unilateral normal contact force $F_N$ and a tangential contact force $F_T$. The simple rheological model for the normal contact force consists of an elastic- plus a viscous contribution as functions of the contact deflection $h_N \geq 0$ and its time rate, respectively:

$$F_N = K_N h_N + \alpha_N \dot{h}_N.$$
The tangential contact force is computed as the elastic response to the relative contact sliding $h_T$ and is bounded by Coulomb-friction, i.e.,

$$F_T = K_T h_T, \quad F_T \leq \mu F_N,$$

where $\mu$ is the contact-friction coefficient. We neglect any volume actions but inertial ones.

At the virgin state, the disk assembly fills a rectangular cell, approximately square, aligned along directions 1 (lateral) and 2 (axial). The cell can undergo generic affine deformations in order to accommodate the most general deformation of a granular REV under small strains. Bi-periodic boundary conditions are implemented according to the Parrinello-Rahman and Lees-Edwards techniques for molecular dynamics \cite{10, 11}. The components of the Cauchy stress tensor $\sigma$ can be retrieved at any time either from inter-particle forces inside the REV, via the classical Love formula, or by simple averages on inter-particles forces across the cell boundaries. Quasi-static conditions being ensured in our tests, the two procedures provide sensitively the same measurements. The components of the infinitesimal strain tensor $\epsilon$ are obtained by a direct quantification of the affine deformation of the bounding periodic cell. The loading history of the generic specimens to be tested against stress probes consists of a standard biaxial compression procedure, with a first stress-rate-controlled isotropic compression and a subsequent axial compression at constant axial strain-rate and constant value $P$ of the lateral pressure $\sigma_{11}$.

The biaxial tests executed for this study can be classified with respect to a small comprehensive number of non-dimensional parameters taking into account material properties and test conditions: (i) the stiffness parameter $\kappa = K_N / P$, setting the scale of contact deflections; (ii) the contact friction coefficient $\mu$; (iii) the damping parameter $\zeta = \alpha N / \sqrt{2 K_N m}$ (with $m$ the mass of the typical particle of diameter $d$) discriminating the underdamped- from the overdamped regime of an elementary oscillator connecting two particle of mass $m$ by a spring of constant $K_N$; (iv) the inertia parameter $\gamma = \dot{\epsilon}_{22} \sqrt{m / P}$, setting the scale of inertia forces. In our study we set $K_T = K_N$ and fix $\mu = 0.3$ for sake of simplicity. We choose $\zeta = 0.9$ in order to keep particle interactions slightly overdamped and so accelerate the numerical convergence. The inertia parameter $\gamma$ is bound to $10^{-4}$, to ensure quasistatic conditions of testing. Finally, the stiffness parameter $\kappa$ takes the values $10^3$, $10^4$ and $10^5$. This first set of parameters controlling the condition of biaxial testing can be extended by introducing the stress ratio $\zeta = Q / P$, where $Q$ is the value of axial pressure $\sigma_{22}$ at which the specimen is tested against stress probes. This extended set of parameter controls the conditions of stress probing. In the large majority of the tests considered here, the stress probes were applied at the investigation points $\zeta = 1.2$, 1.4, 1.6 and 1.8.

A numerical refinement of the isotropic consolidation procedure (prior to axial loading in biaxial tests) allows to obtain “twin” specimens that are macroscopically undistinguishable, namely in terms of stress $\sigma$ and solid fraction $\Phi$, but differ in terms of texture \cite{12, 13, 14}. As shown in Table 1, we apply here this procedure in order to im-
Table 1: Biaxial test families and values of variable parameters.

<table>
<thead>
<tr>
<th>Family</th>
<th>$\kappa$</th>
<th>$\varsigma$ (ca.)</th>
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<td>A3</td>
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<td>1.2, 1.4, 1.6, 1.8</td>
</tr>
<tr>
<td>A4</td>
<td>$10^4$</td>
<td>1.2, 1.4, 1.6, 1.8</td>
</tr>
<tr>
<td>A5</td>
<td>$10^5$</td>
<td>1.8, 1.9</td>
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<tr>
<td>B3</td>
<td>$10^3$</td>
<td>1.2, 1.4, 1.6, 1.8</td>
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<tr>
<td>B4</td>
<td>$10^4$</td>
<td>1.2, 1.4, 1.6, 1.8</td>
</tr>
<tr>
<td>B5</td>
<td>$10^5$</td>
<td>1.2, 1.4, 1.6, 1.8</td>
</tr>
</tbody>
</table>

prove the variety of the population of our specimens. Biaxial tests of type A4 and B4, for example, share the same stiffness parameter $\kappa = 10^4$, but the tests in the first family were “numerically lubricated” during the isotropic consolidation by temporarily dimming $\mu = 0$, which lead to much larger, almost maximal, values of the coordination number $z$ (about 4, vs. 3 ca. for a specimen of type B4). The same difference can be acknowledged between tests of the type A3 and B3 (both for $\kappa = 10^3$) or A5 and B5 ($\kappa = 10^5$, resp.).

Typical axial loading curves are shown in Fig 1 for biaxial tests of type A3, A4 and A5. At small strains, comparing different curves at equal stress ratio $\varsigma$, the axial strain scales with $\kappa^{-1}$, indicating that the contact deformation drives the macroscopic response [12]. Fig 2 refers to axial compression in biaxial tests of type B3, B4 and B5. The inherent microscopic mechanism of deformation at small strains is now the continuous network rearrangement by microscopic instabilities, which makes the macroscopic behaviour actually independent from the contact deformations and therefore almost insensitive to the stiffness parameter $\kappa$: the loading curves superposes at small strains.

3 Incremental response under biaxial loading conditions

The values of stress ratio in Table 1 indicate the investigation points for the stress probing procedure, depending on the biaxial test family. At least two specimens from each family were submitted to parallel tests, in order to assess the degree of repeatability, which was found satisfactory. The stress probes were applied along sixteen different directions, uniformly distributed in the plane of principal stresses (from “0A” to “0P” in Fig. 3). Along each stress direction we applied twelve stress increment levels, corresponding to as many multiples of $2\sqrt{2} P \times 10^{-3}$. The anelastic (supposedly-plastic) strain increments $\delta \epsilon^P$ were obtained by computing the difference

$$\delta \epsilon^P = \delta \epsilon - \delta \epsilon^E$$

between the total strain increments $\delta \epsilon$ and the elastic strain increments $\delta \epsilon^E$. The validity of the partition hypothesis (Eq. 1) is checked here a posteriori, by giving evidence of a plastic flow rule and a yield criterion, as detailed in the following paragraphs where we will be focusing on results from stress probing on specimen issued from biaxial tests of
Figure 1: Normalised deviatoric stress vs. axial strain and volumetric strain vs. axial strain for typical biaxial tests of type A3, A4 and A5.

Figure 2: Normalised deviatoric stress vs. axial strain and volumetric strain vs. axial strain for typical biaxial tests of type B3, B4 and B5.
type A4 and B4. We will finally point out the main differences with respect to other families of specimens, when relevant.

The elastic strain increments cannot be observed directly and were systematically computed according to the assigned stress increments via an elasticity tensor built by assembling the contribution of the contact stiffnesses across the contact network [14]. As an example, in Fig. 4 we represent the incremental elastic response of a specimen of type A4 to the stress probes in Fig. 3, applied at the investigation points \( \varsigma = 1.2 \) and \( \varsigma = 1.8 \). The specimen exhibits a marked elastic anisotropy, slightly evolving during the axial loading.

For the same specimen and investigation points, Fig. 5 shows the plastic strain increments \( \delta \epsilon^P \) computed according to Eq. 1 and compared to the elastic strain increments. The plastic strain increments align neatly along a plastic flow direction in the plane of principal strains. The inclination of such direction with respect to the \( \epsilon_{11} \) axis ranges from 132° (for \( \varsigma = 1.2 \)) to 138° (for \( \varsigma = 1.8 \), resp.). A plastic flow direction is clearly identified also for specimens from biaxial tests in the family B4, as shown in in Fig 6 for the investigation point \( \varsigma = 1.8 \). The inherent plastic flow direction, measured by an angle of 142° with respect to the \( \epsilon_{11} \) axis, is approximately the same as the homologue case in Fig. 5, but the plastic strain increments are about one order of magnitude larger. The elastic contribution appears now negligible in comparison. It is interesting to remark how the plastic strain increments in Fig. 5 group in segments along the plastic flow direction, consistently with the leading deformation mechanism for this type of specimens, by alternate instabilities and rearrangement of the contact network (cf. Sec. 2).

Qualitatively-similar features or the same features where observed for all tested specimens: (i) a clear plastic flow direction can always be identified; (ii) compared to plastic
strain increments, the contribution of the elastic increments tends to reduce with increasing values of the stress ratio and of the stiffness parameter; (iii) such contribution is much weaker, in some cases negligible, for low-coordination specimens (i.e., from families B3, B4 and B5).

We now consider the flow rule

\[
\delta \epsilon^P = \begin{cases} 
\frac{1}{E_P} (\delta \sigma \cdot \xi) \pi & \text{if } f(\sigma) = 0 \text{ and } \delta \sigma \cdot \xi \geq 0 \\
0 & \text{if } f(\sigma) = 0 \text{ and } \delta \sigma \cdot \xi < 0 \\
0 & \text{if } f(\sigma) < 0
\end{cases}
\]

(2)

where the second-order tensor \(\pi\) (\(\|\pi\| = 1\)) represents the plastic flow direction discussed previously, \(E_P\) is the plastic stiffness modulus and the second-order tensor \(\xi\) (\(\|\xi\| = 1\)) identifies the outward-oriented normal to the yield locus seen here as an hyper-surface in the associated stress space. It is worth recalling that these three quantities should not depend on the applied stress increment, but only on the actual state variables. The directional issue, i.e. that of the existence of a plastic flow direction \(\pi\), has just been settled and in order to validate the flow rule one just needs to exhibit a satisfactory fitting of the numerical data with Eq. 2 in norm. A plot of this type is shown in Fig. 7 for the four investigation points of a biaxial test in the family A4. The norm \(\|\delta \epsilon^P\|\) of the plastic strain increments is plotted against the component of the respective stress increments \(\delta \sigma\) along \(\xi\). The plot takes into account only positively-oriented stress increments (i.e., such that \(\delta \sigma \cdot \xi \geq 0\)) and all the stress increment amplitudes are represented, undistinguished. Following Eq. 2, for small-enough stress increments, the four curves should conform to as

Figure 4: Elastic response for a specimen at stress ratio \(\varsigma \simeq 1.2\) (left) and \(\varsigma \simeq 1.8\) (right) from a biaxial test of family A4.
Figure 5: Elastic vs. plastic response of a specimen at stress ratio $\varsigma = 1.2$ (inner frame) and $\varsigma = 1.8$ (outer, resp.) from a biaxial test of family A4.

Figure 6: Elastic vs. plastic response for a specimen at stress ratio $\varsigma = 1.8$ from a biaxial test of family B4.
many straight lines passing by the origin of the plot. In practical terms, the appropriate size of the stress increments should not exceed the range put in evidence by the frame in the figure, out of which the measurements deviate substantially from a linear relation. The suggested range corresponds roughly to the eighth level of stress increment amplitudes in Fig. 3. According to the results obtained insofar from specimens of type A3, A4 and A5, this range seems also to depend sensitively on stiffness parameter $\kappa$: the higher its value the smaller the maximal allowed relative amplitude $\|\delta\sigma\|/P$ of the stress increments for an efficient fitting of the flow rule.

On the other hand, the stress increments cannot be chosen arbitrarily small. A first technical but obvious reason is that they cannot be assigned at the scale set by the accuracy of the numerical algorithm. A second reason appears from Fig. 7, in which the dashed line interpreting the plot for $\varsigma = 1.8$ gives evidence of a slight offset from the origin. This feature, appearing systematically for this type of specimens, might be interpreted as a parasite effect of the specimen preparation procedure. After the investigation point was reached during the axial compression, the numerical simulation was continued, at constant stress, for the time needed to reach a finely-equilibrated configuration, in order not let dynamical effects interfere with the response to stress probes. The observed offset might therefore be seen as a restored minimal elastic region, close to the origin of the plot, due to a slight unavoidable rearrangement of the contact network and consequent loss of plastic memory during the “creep” transition before stress probing.

The values measured on the horizontal axis in Fig. 7 depends on the choice of the quantity $\xi$, i.e., of the outward-orient normal to the yield locus. The direction $\xi$ of the stress space selects the component of the stress increment that is retained as “active” by the flow rule. Arbitrary choices of $\xi$ produce extremely scattered plots, and meaningful curves can only be obtained when $\xi$ points at a precise direction of the stress space. The existence of this particular direction is an implicit, final confirmation of the validity of the flow rule in Eq. 2. Moreover, the minimisation of the plot scattering proves also to be a robust procedure for the detection of the normal to the yield locus. We refer the interested reader to Ref. [9] for systematic measurements of $\xi$ quantity and the plastic flow direction $\pi$ in the whole range of parameters and specimen families considered in this work. We anticipate that those measurement confirm the non-associative character of the flow rule, which is a classical result in granular plasticity. We finally remark that the same qualitative observation concerns the specimen from biaxial tests of type A3 and A5.

The case of a specimen from biaxial tests of type B4 is represented in Fig. 8, where the main differences with respect to the case A4 can be found by looking at the plot for the investigation point $\varsigma = 1.8$. The latter can be observed in more detail as it sets the scale of the vertical axis. The staircase shape of the plot is consistent with the leading deformation mechanisms for specimens from biaxial tests in the families B3, B4 and B5, that deform by repeated instabilities and rearrangements of the contact network. This observation is in accordance with the analogous remark on Fig. 6. Practically speaking, in
order to get meaningful measurements of the plastic stiffness modulus $E^P$ for specimens of this type, one needs to set the order of magnitude of the stress increments at a larger scale, at which the segmentation of the plot is averaged out. The result of this rescaling is suggested in Fig. 9 which results from the application of stress increments of four different amplitudes, for as many multiples of $2\sqrt{2}P \times 10^{-3}$, roughly one order of magnitude higher than those in Figs. 7 or 8.

4 Conclusions

We have presented a robust numerical method, via DEM simulations, for the measurement of the incremental response of model (2D) granular materials. The numerical implementation of this technique, called stress probing, was first proposed by Bardet in 1989 and is now being considered with growing interest by several authors, in particular for the assessment of the basic features of granular elastoplasticity. In this work, those features were studied in a wide range of material properties (in particular the contact stiffness) and for different deformation regimes (either driven by contact deformation or by network rearrangement). By this method, the validity of the partition hypothesis for the deformation response into separate elastic- and plastic contributions can be clearly assessed; under biaxial loading conditions, the plastic incremental response obeys closely a standard non-associated flow rule with well defined plastic flow direction and yield criterion. A key point for an effective application of the method was clearly the proper choice of the range of stress increments amplitudes for the stress probes, depending on the inherent material properties and deformation regimes.
Figure 8: Plastic strain increment amplitude vs. active part of the stress increments for specimens at stress ratios $\varsigma \simeq 1.2$ to 1.8 from a biaxial test of family B4. Stress increment amplitudes from $2\sqrt{2}P \times 10^{-3}$ to $12 \times 2\sqrt{2}P \times 10^{-3}$.

Figure 9: Plastic strain increment amplitude vs. active part of the stress increments for specimens at stress ratios $\varsigma \simeq 1.2$ to 1.8 from a biaxial test of family B4. Stress increment amplitudes from $2\sqrt{2}P \times 10^{-2}$ to $4 \times 2\sqrt{2}P \times 10^{-2}$. 
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PROGRESSIVE FAILURE MECHANISMS IN JOINTED ROCK:
INSIGHT FROM 3D DEM MODELLING

LUC SCHOLTES* AND FREDERIC V. DONZE*†

* Earth Science and Resource Engineering
CSIRO
Queensland Centre for Advanced Technologies, Pullenvale, QLD, Australia
† Laboratoire Sols-Solides-Structures et Risques
UJF-INPG-CNRS
Domaine Universitaire, BP 53, 38041 Grenoble Cedex 9, France
e-mail: frederic.donze@hmg.inpg.fr

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Abstract. Instabilities occurring in rock masses are generally related to the presence of pre-existing discontinuities and the destabilization process often related to the complex interaction between the discontinuities and the rock matrix through the progressive breakage of rock bridges. A 3D model for fractured rock is presented here. The model uses a discrete representation of the intact medium over which discontinuity planes can be overlaid to represent predefined DFNs representative of pre-existing geological structures. These structures, or joints, can then be simulated using a modified contact logic where interactions are setup depending on the orientations and mechanical properties of the joint surfaces. Uniaxial compression tests on a pre-flawed sample are simulated in order to emphasize the relevance of the model in reproducing the so-called “wing crack” extensions usually observed around penny shaped cracks. The model capabilities in terms of crack propagation and coalescence are then discussed on the basis of simulations performed at the scale of a jointed rock slope, with an emphasis on its capability to reproduce one of the key mechanisms usually involved in the development of progressive failure surfaces, the so-called step-path failure mode.

1 INTRODUCTION

Instabilities occurring in rock slopes are generally related to the presence of pre-existing discontinuities and the limit equilibrium method involving a representation of the slope as a set of rigid blocks remains the most commonly adopted approach to assess its potential failure [1]. However, back analyses have shown that for numerous cases, non persistent discontinuities (or joints) are involved in the failure process, with the breakage of rock bridges between those joints being mainly at the origin of the rock mass destabilization [1,2,3]. Thus, if in most cases, progressive failure mechanisms of rock bridges lead to global failure, a model for studying rock slope stability should encompass the nucleation or activation of cracks within the rock, the possible coalescence of which would then lead to the creation of
critical failure surfaces.

Different techniques have been developed to deal with sets of non persistent discontinuities. For example, using stochastic techniques, Einstein et al. [4] made an attempt at relating rock mass stability with persistence in the geometry and spatial variability of discontinuities. However, this approach was based on the limit equilibrium analysis and therefore, remained limited in reproducing and understanding the progressive nature of slope failure. More recently, numerical methods have led to significant enhancements in rock slope stability analysis, which can take into account complex but realistic features (e.g., Discrete Fracture Network, anisotropy, 3D effects, non-linear behaviour, etc…). If classical continuous or discrete approaches in their initial formulation do not seem adapted to describe the progressive failure mechanisms in jointed rock, several attempts have been made to extend their capabilities. For example, Wang et al. [5] demonstrated that the application of a particle flow code can provide valuable insight into the stability analysis of heavily jointed rock slopes. Eberhardt et al. [2] showed that a coupled FEM/DEM formulation [6] can reproduce observed failure mechanisms by taking advantage of both continuous and discrete approaches (case study: 1991 Randa rockslide). However, to our knowledge, all these previous studies were performed in 2D. A step further is therefore to use 3D models which can reproduce the complex combination of intact material fracturing and yielding within discontinuity planes.

Using a discrete approach, a 3D simulator for jointed rock slopes which accepts Discrete Fracture Networks (DFN) has been recently developed by Itasca [7]. Based upon a similar approach, a 3D model implemented into YADE Open-DEM [8] is presented in this paper. The model uses a discrete representation of the intact rock mass, in which DFNs can be plugged in a straightforward way as a set of planes representing discontinuities (joints).

In this paper, it is shown that the model can reproduce typical progressive failure mechanisms as they have been observed both in the laboratory and at the scale of a rock slope. Simulations are presented to show how non persistent discontinuities can interact and induce fracturing within a rock mass.

2 MODEL DESCRIPTION

The numerical formulation of YADE is given in Kozicky and Donze [8]. It is an extensible open-source framework for discrete numerical modelling, focused on the Discrete Element Method. The algorithm used in YADE involves two steps. In the first one, interaction forces are computed when elements slightly interpenetrate each other. In the second step, Newton second law is used to determine, for each DE, the resulting acceleration, which is then time integrated to find the new element positions. This process is repeated until the simulation is finished. The dynamic formulation allows the model to follow highly nonlinear behaviour characteristic of brittle material as a result of local interaction link breakage in both tensile and shear failure modes.

2.1 Intact Rock

The experimental results obtained by Sulem and Ouffroukh [9] on Fontainebleau sandstone provide a characteristic and well referenced data set for an intact brittle rock behaviour and it has been used here to setup the mechanical properties of the intact part of the model. Average values of 5 GPa for Young’s modulus $E$, 0.25 for Poisson’s ratio $\nu$, 41.3° for the internal
friction angle $\Phi$ and 15.5 MPa for the cohesion $C$ were obtained by Sulem and Ouffroukh [9] based on a series of drained triaxial tests. The calibration procedure of the discrete model was thus performed in order to reproduce within a best agreement the macroscopic behaviour of this sandstone. The triaxial curves and rupture envelop predicted by the model are presented in Figure 1.

![Figure 1: Stress Strain curves (a) and rupture envelop (b) obtained from triaxial and uniaxial test simulations performed on the model calibrated to simulate Fontainebleau sandstone after [9].](image)

### 2.2 Discontinuities

In order to model discontinuities in the DEM, a specific contact formulation, related to the work made by Cundall and co-authors for the development of the Synthetic Rock Mass [10], has been implemented into YADE Open DEM. This joint contact logic is based on the identification and reorientation of each DE interaction which crosses the plane representing the discontinuity surface (Figure 2). With this joint contact logic the discontinuities structural effects on the fabric of the medium can be accounted for and any dependence of the joint behaviour on the DE distribution size is avoided. For instance, using the classical contact logic, the shear resistance is higher when less DEs are involved in the joint due to the interlocking of the DEs (Figure 2a). Indeed, the degree of interlocking and the associated roughness increases when the ratio between the size of the DE and the effective joint surface decreases. The resulting shear strength of the joint is therefore dependent on the resolution of the model. On the contrary, the enhanced contact logic provides a constitutive behaviour of the joint model which is fully controlled and determined by its local mechanical properties and which does not depend on the resolution of the model as illustrated in Figure 2b for a case without any cohesion for which perfect elastic-plastic behaviour is expected. In addition to the possibility to introduce cohesion in the joint model, dilation can also be accounted for in order to match the actual properties of the simulated joint in a more realistic manner.
3 CRACK INITIATION AND PROPAGATION

A classical problem which has to be addressed when dealing with the progressive failure of a rock mass is to verify that the model is capable of reproducing the expected wing cracks developing at the tips of an existing fracture under compressive loading. This problem has been extensively studied in the last fifty years with numerous attempts aiming at understanding the mechanisms at the origin of crack initiation and growth into the intact medium [11].

To assess the ability of the model to tackle this problem, a uniaxial compressive test simulation has been performed on a prismatic sample containing a pre-defined frictionless disk shaped crack oriented at 45 degrees from its principal axis.

In the model, local rupture (micro-cracking) appears when the cohesive interaction between two DE reaches its tensile limit and micro-cracks are represented as disks for which the normal orientation corresponds to the actual tensile loading direction. It is the coalescence of those micro-cracks which then produces macroscopic failure surfaces inside the medium. As presented in Figure 3, the typical wing crack pattern resulting from stress concentration at the fracture circumference and the subsequent coalescence of local micro-cracks can be properly reproduced by the proposed model and is in good agreement with the experimental observations made by Dyskin and co-authors [11].
Luc Scholtes and Frederic Victor Donze.

Figure 3: Crack distribution (“wing crack”) induced by uniaxial compression of a pre-flawed sample: (a) experiment on Plexiglas from [12], (b) model prediction.

4 SLOPE STABILITY

In order to present the model capabilities in a clear way, 3D slices of a slope have been used in this study (see Figure 4(a)). The slope model consists of a set of 66,000 DE linked by more than 330,000 cohesive links (Figure 4). The face slope angle is equal to 80°. The DEs can move in all directions except for the ones lining the boundaries (see Figure 4(b) for details). A gravity induced stress is applied to the model before every simulation. DE density is chosen such that the gravity induced vertical stress $\sigma_v$ at the bottom boundary corresponds to the one expected for a 50 m high slope consisting of a 2500 kg/m$^3$ rock density (in this case, $\sigma_v \approx 1.3$ MPa). In this study, the joint properties are chosen to simulate cohesionless joint planes presenting a 30° friction angle and a dilation angle of 10° and the intact medium properties calibrated according to section 2.1 to reproduce the behaviour of Fontainbleau sandstone as described by [9]. Additionally, the stiffness is 10 times smaller for the interactions located across the joint planes than for the ones inside the rock matrix.

Figure 4. (a) Three dimensional slice of a slope used in this study, (b) boundary conditions (for sake of clarity, results will be mainly represented along the (x,y) plane.

In order to lead the slope model to failure, an iterative scheme has been used which consists in progressively reducing the strength of the intact part of the material, i.e. decreasing
simultaneously the tensile strength and cohesion of the local interaction links. The strength reduction process is active as long as the crest of the slope stays in a stable or quasi-static condition. The quasi-static condition is ensured by checking that the velocity of one of the DE belonging to the crest corner is lower than a predefined value (0.1 mm/s here).

The simulations presented in the following were conducted on a 64-bit Intel Quad Core 2.6GHz preprocessor computer with 8 MB RAM. Each of them was run in about 3 hours.

4.1 Step-Path Failure

The following results present study-cases where pre-existing joints are not restrained to major failure surfaces, but are rather randomly distributed inside the medium. Two configurations were set up with joint sets dipping respectively at 40° and 80° inside the slope (see Figures 5 and 6). A first remarkable difference between these two configurations is that, contrarily to the sub-horizontal joint set (dip 40°), destabilization of the slope crest only occurred after a very high degradation level of the intact material for the sub-vertical one (dip 80°). Moreover, the resulting failure patterns are totally different depending on the joint set orientation. Indeed, if the sub-horizontal joint set leads to a typical en-echelon failure due to the appearance of bridging cracks caused by sliding on the pre-existing fractures, the sub-vertical discontinuities do not seem to influence the failure of the slope, with a circular failure surface appearing near the slope face, as typically observed in homogeneous slopes.

![Figure 5](image1.png)  
**Figure 5.** Cracks (left) and displacement field (right) induced by strength degradation in the case of a random joint set with a 40° dip angle.

![Figure 6](image2.png)  
**Figure 6.** Cracks (left) and displacement field (right) induced by strength degradation in the case of a random joint set with a 80° dip angle.
Despite their relative simplicity, both examples nevertheless clearly show the model capabilities in terms of failure surface prediction with respective descriptions of critical path failure through breakage of intact rock bridges, and circular failure surface characteristic of homogeneous slopes.

In order to complete a simulation of a more realistic rock slope destabilization process, a slope model has been constructed which includes both 40° and 80° joint sets. Final crack patterns and displacement field are presented in Figure 7.

Even though it has been restricted to a particular joint set configuration, the model shown here can reproduce the complex interaction occurring between pre-existing natural discontinuities and fracture propagation in intact rock. The failure surface typically develops along a critical path involving both fracture propagation inside intact rock and sliding along discontinuity planes, resulting in the destabilization of the upper part of the slope. In addition, a secondary failure surface can be observed that has developed at a deeper level inside the slope. It has to be noted that, at the final stage of the simulation, the corresponding secondary block did not collapse since the degradation process was stopped after the first block destabilization. However, it is clear that this secondary block consists of a potentially unstable rock mass which would certainly destabilize after any additional perturbation of the slope.

![Figure 7. Cracks (left) and displacement field (right) induced by strength degradation in the case of 2 random joint sets with respective 40° and 80° dip angles.](image)

**8 CONCLUSIONS**

The aim of the present paper is to present a Discrete Element Method dedicated to the simulation of fractured rock masses using a particle-based approach. YADE is a general 3D DEM open source package which has been used to study the stability of fractured media with an explicit representation of both the intact part of the material and the pre-existing structural discontinuities.

From laboratory scale simulations to slope stability case studies, the examples presented in this paper show that this method can investigate the complex behaviour of unstable fractured rock masses: the combined effect of pre-existing discontinuities on the elastic properties and strength of a rock mass as well as the possibility to follow the evolution of the fracturing mechanisms involved in the failure process promises new perspectives in slope stability
analyses. Distinct configurations can be generated in order to discriminate the respective roles of the geological structures regarding the mechanical properties of both the intact rock and the discontinuities. Some new insights can also be gained concerning the effect of joint persistence and orientation on the destabilization process of jointed rock slopes.

The use of the model combined with the use of suitable field mapping techniques, would then provide relevant information for the establishment of appropriate safety plans by clarifying the potential failure mechanisms associated to the rock structure.

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QUASISTATIC GRANULAR MATERIAL RHEOLOGY
FROM PARTICLE SIMULATIONS

J.-N. ROUX
Université Paris-Est, Laboratoire Navier, 2 Allée Kepler, Cité Descartes, 77420 Champs-sur-Marne, France.
E-mail: jean-noel.roux@ifsttar.fr

Key words: granular materials, elastoplasticity, stress-strain behaviour

Abstract. We report on the quasistatic behaviour of model granular materials, as probed by DEM simulations of isotropic compression and triaxial compression tests, focussing on the macroscopic behaviour dependence on control parameters expressed in dimensionless forms that combine contact laws with test conditions, and on the influence of the initial state. A discussion of the microscopic origins of strain, which in some situations of small strains and stable contact networks are due to contact deflections, and in other cases results from the continuous breaking and repairing of networks under varying loads provides a useful classification of rheological regimes. Some guidelines for parameter choices in numerical simulations, and for some homogenization approaches, are inferred.

1 INTRODUCTION

Discrete element simulations of granular systems have become a widespread approach, but its implementation requires adequate choices for many parameters. The mechanical properties of quasistatically deformed granular assemblies strongly depend on initial packing geometry. This communication is a contribution to the classification of initial states and quasistatic rheological regimes, based on simple state variables and dimensionless numbers, combining contact laws with externally imposed conditions. It addresses such issues as the sensitivity to contact stiffness and the rigid grain limit, the approach to the quasistatic limit and the effect of the initial coordination number, in addition to the initial density, on small to moderate strain response to deviator stresses (Sec. 3). First, Sec. 2 discusses possible states of isotropic packings and their response to isotropic compression. Sec. 4 lists a few remarkable conclusions.
2 MODEL MATERIAL AND SIMULATION PROCEDURE: ASSEMBLING STAGE AND COMPRESSION

We focus here on grain-level numerical simulations of the isotropic compression and the triaxial compression tests of assemblies of identical spherical beads, as in Refs. [1, 2, 3, 4]. Isotropic compression [5] is interesting both in itself and because it is a necessary preparation step, in simulations as well as in the laboratory, before a specimen is subjected to deviatoric loads and its internal shear resistance is probed.

2.1 Material definition, contact laws

We consider assemblies of $N=4000$ beads of diameter $a$, interacting at their contacts with (simplified) Hertz-Mindlin elasticity [6] and Coulomb friction, with coefficient $\mu$ (equal to 0.3, unless otherwise specified). Thus the normal elastic force $F_N$ in contacts, assuming beads are made of an elastic material with Young modulus $E$ and Poisson ratio $\nu$, relates to the normal contact deflection, $h$, as $F_N = \frac{E\sqrt{a}}{1-\nu^2}h^{3/2}$ and the tangential force $F_T$ varies incrementally with tangential relative displacement $u_T$ at contacts as $dF_T = K_TdF_N$, involving stiffness parameter $K_T = \frac{2-2\nu}{2-\nu}\frac{dF_N}{dh}$, and subject to the Coulomb requirement $||F-T|| \leq \mu F_N$. These relations should be supplemented by additional conditions ensuring thermodynamic consistence [7] and objectivity [8], as detailed in [3].

In order to damp out oscillations and accelerate the approach to mechanical equilibrium, some additional viscous forces in contacts might be introduced.

When a confining pressure $P$ is applied, the deformation within grains in the contact regions is conveniently assessed by the stiffness number $\kappa = \left[ \frac{E}{(1-\nu^2)P} \right]^{2/3}$ (contact deflections $h$ are $\propto \kappa^{-1}$ [3]). For glass beads with $E = 70$ GPa and $\nu = 0.3$, the values used in the simulations reported in the sequel, one has $\kappa \simeq 8400$ for $P = 100$ kPa. Another important dimensionless control parameter is the inertial number, which is an indicator of the importance of dynamical effects in systems out of equilibrium. It is defined as $I = \dot{\varepsilon}\sqrt{\frac{m}{aP}}$ for grains of mass $m$ when the macroscopic strain rate is $\dot{\varepsilon}$ [9, 2, 3, 10]. $I$ is the ratio of inertial to deformation characteristic times. The quasistatic limit is simply defined as $I \rightarrow 0$.

It is convenient to implement fully periodic boundary conditions in all three directions and to perform partly stress-controlled tests. Stress components are evaluated in a specimen of volume $\Omega$ with the usual formula involving a sum over all contacts between pairs of particles $i, j$, where the contact force is $F_{ij}$ and the branch vector $r_{ij}$ points from the...
Table 1: Isotropic states, with $\mu = 0.3$ ($\kappa \simeq 39000$ for A and C, $\kappa \simeq 181000$ for B and D), obtained with different assembling procedures.

<table>
<thead>
<tr>
<th>Procedure</th>
<th>$\Phi$</th>
<th>$z^*$</th>
<th>$x_0$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A ($\mu_0 = 0$)</td>
<td>0.6370 ± 0.0002</td>
<td>6.074 ± 0.0015</td>
<td>1.3 ± 0.2</td>
</tr>
<tr>
<td>B ($\mu_0 = 0.02$)</td>
<td>0.6271 ± 0.0002</td>
<td>5.80 ± 0.007</td>
<td>1.95 ± 0.02</td>
</tr>
<tr>
<td>C (vibrated)</td>
<td>0.635 ± 0.002</td>
<td>4.56 ± 0.03</td>
<td>13.3 ± 0.5</td>
</tr>
<tr>
<td>D ($\mu_0 = \mu = 0.3$)</td>
<td>0.5923 ± 0.0006</td>
<td>4.546 ± 0.009</td>
<td>11.1 ± 0.4</td>
</tr>
</tbody>
</table>

center of $i$ to the center of $j$, as

$$\sigma_{\alpha\beta} = \frac{1}{\Omega} \sum_{i<j} F_{ij}^{(\alpha)} r_{ij}^{(\beta)}$$  \hspace{1cm} (1)

(if direct momentum transport due to particle velocities can be neglected). The dimensions of the simulation cell satisfy dynamical equations in order to impose prescribed values to some diagonal components of tensor $\sigma$ [3, 10, 11].

2.2 Initial states

In the assembling stage, a granular fluid is prepared at relatively low solid fraction (e.g., $\Phi = 0.45$, below hard sphere crystallization density $\Phi \simeq 0.49$) and randomized as a hard sphere (energy conserving) liquid, via an event-driven method. Then, an isotropic pressure is applied. In this first and all subsequent isotropic compressions, the system is requested to equilibrate under preset values of the applied pressure, with the condition that the strain rate should never exceed a certain threshold. In order to obtain different initial state densities and structures, one may use a different friction coefficient $\mu_0$ in the initial sample preparation stage. Table 1 gives the basic characteristics of equilibrated packings built under low isotropic confining pressure (high $\kappa$): solid fraction $\Phi$, fraction of “rattlers” (grains carrying no load) $x_0$, coordination number $z^*$ of non-rattlers. A samples are built without friction ($\mu_0 = 0$), a well known procedure to obtain samples with the “random close packing” density [3], B ones are prepared with $\mu_0 = 0.02$, this small level of friction entailing a notable density change. D states are built with the final friction coefficient $\mu = 0.3$ acting in the granular gas stage ($\mu_0 = \mu = 0.3$), while compression is carried out slowly ($I \leq 10^{-3}$). Finally, C systems are assembled from A ones, after a slight dilation, strong vibrations, and recompaction to jamming with $\mu = 0.3$. Remarkably, they are nearly as dense as A ones, but with a low coordination number and a large population of rattlers.

2.3 Isotropic compression and pressure cycles

The results of the isotropic compression of the bead packs of Tab. 1 are shown in Fig. 1. The pressure dependence of solid fraction $\Phi$ in a compression cycle is nearly reversible (e.g., the initial small difference in density between A and C systems is retrieved), but the
internal structure might be strongly affected, as the initially high coordination number in systems A and B decreases upon unloading to low values (as in C and D).

2.4 Samples assembled with cohesion

In the presence of attractive forces in the contacts, much looser structures may be stabilized [12], provided the initially agitated particles of a granular gas are allowed to stick and form tenuous aggregates before the system is subjected to an external pressure. Fig. 2 displays a typical compression curve of an initially loose pack of beads with capillary cohesion, due to small menisci forming at intergranular contacts. Such an attractive force, with a meniscus of volume $V$ joining two spheres of diameter $a$ separated by distance $D$, 

![Figure 1: Effect of isotropic pressure cycle (from 10 to $10^4$ kPa, and back down to 10 kPa) on samples of Tab. 1. Left: solid fraction $\Phi$; right: coordination number of non-rattlers, $z^*$.](image1.png)

![Figure 2: Effect of pressure cycle on system with capillary cohesion, similar to Fig. 1. Left: $\Phi$ (cohesionless results recalled for comparison) versus $P$; right: coordination number, of contacts $z_c$(bottom), of menisci, $z_m$(top), versus reduced pressure $P^*$.](image2.png)
is conveniently approximated \[13\] as

\[ F_c = F_0 \left[ 1 - \left( 1 - \frac{4V}{\pi aD^2} \right)^{-1/2} \right], \quad \text{with} \quad F_0 = \pi \gamma a, \quad (2) \]

where \( \gamma \) is the surface tension and perfect wetting (zero contact angle) is assumed. These data correspond to volume \( V = 10^{-3} a^3 \) attributed to menisci that form when grains come into contact and break in receding pairs separated by distance \( V^{1/3} \) \[13\]. The relative importance of cohesive forces and confining stress is expressed by dimensionless reduced pressure \( P^* = a^2 P/F_0 \) \[12\]: loose structures stabilized by attractive forces survive as long as \( P^* \) is small enough, and collapse as soon as the confining stress starts to dominate. The pressure cycle (Fig. 2) entails a large irreversible density increase, in which the contact coordination number hardly changes unless \( \kappa \) (Fig. 1) decreases too much. As cohesive forces become negligible under high \( P^* \), they might be removed (as if wet grains were dried) with no effect on the subsequent density curve upon unloading (Fig. 2). The resulting cohesionless packing is looser than the loosest ones assembled with no cohesion (D in Tab. 1). Its coordination number and rattler density are similar to the values of states C or D of Table 1.

3 SIMULATIONS OF TRIAXIAL COMPRESSION

Triaxial compression tests are simulated with the standard procedure in which the axial strain rate \( \dot{\epsilon}_a \) is kept constant. The deviator stress, \( q \), is measured, as a function of axial strain \( \epsilon_a = \epsilon_1 \), as \( q = \sigma_1 - \sigma_3 \), where \( \sigma_1 \) is the major (“axial”) principal stress conjugate to \( \epsilon_a \), while the other two (lateral) principal stresses \( \sigma_2 = \sigma_3 \) are kept equal to the initial isotropic pressure \( P \). The simulations reported here compare dense states A (high coordination number) and C (low coordination number). Pressure values, assuming particles are glass beads, vary between 10 kPa (\( \kappa = 39000 \)) and 1 MPa (\( \kappa = 1800 \)).

We first check for the approach of the quasistatic and the macroscopic limit in 3D, strain-rate controlled DEM simulations, then discuss the influence of coordination number, and sensitivity to stiffness parameter \( \kappa \).

3.1 Reproducibility, quasistatic limit

Fig. 3 checks for stress-strain curve reproducibility in both A and C cases, for small axial strains. Thanks to the fully periodic boundary conditions \[3\], the macroscopic mechanical behavior is quite well defined with \( N = 4000 \). The approach to the quasistatic limit can be assessed on checking for the innocuousness of the dynamical parameters, i.e., inertial number \( I \), and reduced damping parameter \( \zeta \). \( \zeta \) is defined as the ratio of the viscous damping constant in a contact to its critical level, given the instantaneous value of the stiffness constant. We found it convenient to use a constant value of \( \zeta \) in our simulations, as in \[3\]. Fig. 3 also shows that provided inertial number \( I \), characterizing dynamical effects, is small enough, both \( I \) and \( \zeta \) become irrelevant. Fig. 3 shows that the quasistatic
Figure 3: Left: small strain part of $q(\epsilon_a)$ curves for 5 different samples of each type, A (top curves) and C (bottom ones) with $N = 4000$ beads. Right: $q(\epsilon_a)$ and $\epsilon_v(\epsilon_a)$ curves in one type C sample for the different values of $\zeta$ and $I$ indicated.

limit is correctly approached for $I \leq 10^{-3}$, quite a satisfactory result, given that usual laboratory tests with $\dot{\epsilon}_a \sim 10^{-5}$ s$^{-1}$ correspond to $I \leq 10^{-8}$.

3.2 Influence of initial coordination number

Fig. 4 compares the behavior of initial states A and C, in triaxial compression with $P = 100$ kPa ($\kappa \approx 8400$). Although, conforming to the traditional view that the peak

Figure 4: $q(\epsilon_a)$ (left scale) and $\epsilon_v(\epsilon_a)$ (right scale) curves for A and C states under $P = 100$ kPa. Averages over 5 samples of 4000 spherical grains.

deviator stress is determined by the initial sample density, maximum $q$ values are very nearly identical in systems A and C, the mobilization of internal friction is much more gradual for C. For A, the initial rise of deviator $q$ for small axial strain is quite steep, and
the volumetric strain variation becomes dilatant almost immediately, for \( \epsilon_a \sim 10^{-3} \). In [4] it was shown that measurements of elastic moduli provide information on coordination numbers. It is thus conceivable to infer the rate of deviator increase as a function of axial strain from very small strain (\( \sim 10^{-5} \) or below [14, 4]) elasticity. Most experimental curves obtained on sands, which do not exhibit \( q \) maxima or dilatancy before \( \epsilon_a \sim 0.01 \), are closer to C ones. However, some measurements on glass bead samples [15] do show fast rises of \( q \) at small strains, somewhat intermediate between numerical results of types A and C.

### 3.3 Influence of contact stiffness

The fast \( q \) increase in a small strain interval (say \( \epsilon_a \leq 5 \times 10^{-4} \)) is sensitive to stiffness level \( \kappa \). This is readily checked on changing the confining pressure. Fig. 5 shows the curves for triaxial compressions at different \( P \) values (separated by a factor \( \sqrt{10} \)) from 10 kPa to 1 MPa, with a rescaling of the strains by the stiffness parameter \( \kappa \), in one A sample. They coincide for \( q/P \leq 1 \): within this wide deviator range, the macroscopic strains scales with contact deflections. This is clear evidence for a strain resulting from deformation at contacts – a regime we refer to as regime I (type I strains). For larger strains, curves separate on this scale, and tend to collapse together if \( q/P, \epsilon_a \) are simply plotted versus \( \epsilon_a \). The strain dependence on stress ratio is independent from contact stiffness. This different sensitivity to pressure is characteristic of a rheological regime we refer to as regime II, in which strains are considerably larger and due to network rearrangement. Fig 5 also shows that it applies to C samples almost throughout the investigated range, down to small deviators (a behavior closer to most usual experimental results on sands than type A configurations). At the origin (close to the initial isotropic state, see inset on

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**Figure 5:** Left: \( q(\epsilon_a)/P \) and \( \epsilon_v(\epsilon_a) \) curves for one A sample and different \( P \) values. Strains on scale \( (P/P_0)^{2/3} \propto \kappa^{-1} \), \( P_0 = 100 \) kPa. Right: \( q(\epsilon_a)/P \) for the same \( P \) values in one C sample. Inset: detail with blown-up \( \epsilon \) scale, straight lines corresponding to Young moduli in isotropic state.
fig. 5, right plot), the tangent to the curve is given by the elastic (Young) modulus of the granular material, \( E_m \), and therefore \( q/P \) scales with \( \kappa \), but curves quickly depart from this behaviour (around \( q = 0.2P \)). The approximately elastic range \([4]\) is quite small, as observed in experiments \([14, 16, 17]\).

As to the isotropic compression tests of Sec. 2, they are obviously in regime I in cohesionless systems, and in regime II for loose cohesive structures.

3.4 Calculations with a fixed contact list

Within regime I, the mechanical properties of the material can be successfully predicted on studying the response of one given set of contacts. Those might slide or open, but the very few new contacts that are created can be neglected. To check this in simulations, one may restrict at each time step the search for interacting grains to the list of initially contacting pairs. Fig. 6 compares such a procedure to the complete calculation. The curve marked “NCC” for no contact creation is indistinguishable from the other one for \( q \geq 0.8 \). We thus check that, in regime I, the macroscopic behavior is essentially determined by the response of a fixed contact network.

3.5 Type I strains and elastic response

Fig. 6 also shows that the small strain response of A samples, within regime I, close to the initial state, is already irreversible: type I strains are not elastic. An approximately elastic behavior is only observed for very small strains, as depicted in the inset of Fig. 5 (right graph). In this small interval near the initial equilibrium configuration, the stress-strain curve is close to its initial tangent, defined by the elastic modulus. Moduli \([4]\) can be calculated from the stiffness matrix of contact networks. One may also check that the unloading curves shown on Fig. 6 comprise a small, approximately elastic part, with the relevant elastic modulus (the Young modulus for a triaxial test at constant lateral stress).
defining the initial slope. At the microscopic level, a small elastic response is retrieved upon reversing the loading direction because contacts stop sliding. The elastic range is strictly included in the larger range of type I behavior.

3.5.1 Fluctuations and length scale

Finally, let us note that regimes I and II also differ by the importance of sample to sample fluctuations: curves in Fig. 3 (left plot) pertaining to the different samples of type A or C are confused as long as \( q \leq 1.1P \) (case A) or \( q \leq 0.3P \) (case C), which roughly corresponds to the transition from regime I to regime II. Larger fluctuations imply that the characteristic length scale associated with the displacement field (correlation length) is larger in regime II. Whether and in what sense rearrangements triggered by instabilities in regime II, in a material close to the rigid limit (large \( \kappa \)), can be regarded as local events is still an open issue.

4 SOME CONCLUSIONS

This brief account of isotropic and triaxial tests on model material for different initial states reveals that the initial states should be classified according to their coordination number in addition to their density, as dense systems might be as poorly coordinated as loose ones. Compression test results are independent of dynamical parameters if the inertia parameter \( I \) is kept small enough. The response to an isotropic compression of cohesionless systems is apparently elastic as density changes are close to reversible, but contact networks exhibit irreversible changes in pressure cycles, with a very notable decrease in coordination number if its original value was large. Cohesion may stabilize loose structure that collapse under growing applied load, and density increase in compression then depend on the maximum value of reduced pressure \( P^* \) in the sample history, rather than on stiffness parameter \( \kappa \). Regime I corresponds to the stability range of a given contact structure. It is larger in highly coordinated systems. It is observed in the beginning of monotonic loading tests, in which the deviator stress increases from an initial isotropic configuration, and also after changes in the direction of load increments (hence a loss in friction mobilization). Strains, for a given stress level, are then inversely proportional to contact stiffnesses. The deviator range in regime I, in usual monotonic tests, is strictly larger than the small elastic range, but strictly smaller than the maximum deviator. It was shown in previous studies of 2D systems [18, 19, 20] not to vanish in the limit of large systems, unlike in the singular case of rigid, frictionless particle assemblies [21, 22]. Regime I is limited by the occurrence of elastoplastic instabilities in the contact network and does not coincide with the prediction of the critical yield approach. In regime I, the work of the externally applied load is constantly balanced by the one of contact forces, so that the kinetic energy approaches zero in the limit of slow loading rates. A remarkable consequence is that the instability condition based on the negativity of the macroscopic second-order work [23] is never fulfilled, as macroscopic and microscopic works coincide,
and the latter is positive. In regime II, network rearrangements are triggered by instabilities and some bursts of kinetic energy are observed [24]. Larger fluctuations witness longer-ranged correlations in the displacements. The microscopic origin of macroscopic strains, which are independent on contact elasticity for usual stiffness levels $\kappa$, lies in the geometry of grain packings.

On attempting to predict a macroscopic mechanical response from packing geometry and contact laws, the information about which kind of strain should dominate is crucial.

REFERENCES


SCALING ANALYSIS OF DEFORMATION FIELD WITHIN GRANULAR MATERIALS: APPLICATION TO STRAIN LOCALIZATION

FLORENT GIMBERT*, GAEL COMBE†, DAVID AMITRANO* AND JEROME WEISS#

*Institut des Sciences de la Terre (ISTerre)
CNRS, Université Joseph Fourrier
Domaine Universitaire
38401 GENOBLE, France
e-mail: florent.gimbert@ujf-grenoble.fr

† Laboratoire Sols, Solides, Structures, Risques (3SR)
UMR 5521 (UJF, INPG, CNRS)
Domaine Universitaire
38041 GRENOBLE Cedex 9, France

#Laboratoire de Glaciologie et de Géophysique de l'Environnement (LGGE)
CNRS, Université Joseph Fourrier
38402 St Matin d'Hères, France

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Abstract. Discrete element method (DEM) simulations using periodic boundary conditions and molecular dynamics are conducted on a frictional granular media. Two dimensional strain controlled biaxial tests are carried out on an assembly of circular particles interacting via elastic contacts and Coulomb friction. The spatial correlations that take place within the deformation field along the loading path are tracked by a scaling analysis of the continuous strain rate field. This method allows us to discuss the degree of strain localization occurring throughout the test. The analysis of the correlation length in the early stages of macroscopic deformation leads to the identification of two distinct behaviors. First, a divergence of the correlation length on the first deformation invariant, i.e. the divergence, is reported at the onset of macroscopic dilation. This suggests an interpretation of the contraction peak as a critical point. Secondly, an increase of the correlation length on the second deformation invariant, i.e. the shear, is also observed before the peak load. However, saturation remains on the scaling law. We argue that this second behavior is associated to macroscopic shear banding: our analysis accurately gives its outbreak on the stress versus strain curve. Finally, a dependence of the correlation length as a function of the deformation window considered is reported. This shows that scaling properties within the deformation field emerge from long range interactions within an assembly of rigid frictional particles.
1 INTRODUCTION

Discrete element numerical simulations (DEM) of granular materials show an extraordinarily rich behavior emerging from simple mechanical interactions at the particle scale.

As shown by Radjai and Roux [1], a homogeneous macroscopic loading applied to a granular material constituted of a random assembly of rigid circular frictional particles leads to the development of large, non-gaussian particle velocity fluctuations at small time scales, as well as a power law decay of the spatial power spectrum of the velocity field. This indicates long-range correlations. Indeed, heterogeneous distribution of contact forces on scales much larger than the typical particle size [2-3] induces collective motions of particle assemblies, i.e. long range correlations, to operate within granular media. Thus, to characterize the mechanical fields (stress, strain) within granular materials from the particle scale to the large scale is of first interest in order to describe and understand properly their macroscopic mechanical response.

Following this route, the objective of this paper is to investigate the spatial correlations that take place within the deformation field of frictional granular materials during compressive loading. Can classical macroscopic features such as dilatancy or shear banding be associated to specific scaling properties of the associated strain field?

The mechanical behavior of disordered cohesive (i.e. non granular) materials, and specifically their approach to final failure, has been widely investigated by the statistical physics community in recent years (e.g. [4-5]) from numerical models such as the random fuse model, the tensorial random spring model or the progressive damage model [6]. Finite size scaling in the power law distributions of avalanche sizes $S$ (defined as the number of broken fibers, bonds or damage events) and energies $E$ have been reported, providing an argument in favor of a critical phase transition interpretation of failure. Recently, from a spatial correlation analysis of damage events as well as a multi-scale analysis of the strain-rate field, Girard et al. [6] reported a divergence of the correlation length as approaching the failure, another strong argument for the critical character of failure.

Following this work, we perform here a coarse graining analysis on the continuous incremental strain field of granular materials at several stages of DEM simulations. This analysis allows a quantitative estimation of the degree of strain localization that take place within the media. Then, the results are interpreted in the framework of statistical physics in order to determine if the macroscopic mechanical features such as the onset of dilatancy or the shear strain softening can be associated to specific scaling laws of the strain-rate field.

2 GRANULAR MODEL

2.1 Microscopic Constitutive laws

The discrete element method involved is one of the most widely used, Molecular Dynamics (MD) [7]. Particles motions are time-discretized with a 3\textsuperscript{rd} order predictor-corrector scheme. All grains interact via linear elastic laws and Coulomb friction when they are in contact: the normal contact force $f_n$ is related to the normal apparent interpenetration $\delta$ of the contact as $f_n = k_n \delta$, where $k_n$ is a normal stiffness coefficient ($\delta > 0$ if a contact is present, $\delta = 0$ if there is no contact). The tangential component $f_t$ of the contact force is proportional...
to the tangential elastic relative displacement, with a tangential stiffness coefficient $k_t$. The Coulomb condition $|f_t| \leq \mu f_n$ requires an incremental evaluation of $f_t$ for each time step, which leads to some amount of slip each time one of the equalities $f_t = \mu f_n$ is imposed. In this study, $k_n$ is such that $K = k_n/\sigma_3 = 1000$ [8]. The stiffness ratio is $k_n = k_t = 1$. Granular assemblies are made of two-dimensional rigid circular grains. Their diameters are uniformly distributed between $D_{\text{min}}$ and $D_{\text{max}} = 3D_{\text{min}}$. Periodic boundary conditions are used [7]. After an isotropic compression without intergranular friction $\mu = 0$, dense samples of initial porosity $\eta_i = 0.15$ are submitted to a vertical compression with keeping the lateral stress $\sigma_3$ constant (biaxial tests). The tests presented in this study consider $\mu = 1$. The vertical constant strain rate $\dot{\varepsilon}_1$ is chosen such that mechanical transformation can be assumed as quasi-static. For that, $\dot{\varepsilon}_1$ is obtained by setting $I = 5 \times 10^{-5}$, where $I$ is the inertial number [8]. Under these considerations, the increment of deformation $\delta \varepsilon_1$ associated to one time step integration is $\delta \varepsilon_1 = 8.5 \times 10^{-9}$.

Figure 1 shows a typical macroscopic stress strain curve obtained on a sample made of 45000 grains. At the beginning of the test, a contracting regime is observed on the volume variation up to an axial strain of about 0.29% corresponding to the onset of dilation: since dense samples are considered here, grains rearrangements in the early stages of deformation are limited and contraction is mainly observed because of an elastic contact description between particles [9]. The inelastic deformation in the contractant regime is due to loss of contact and Coulomb friction between particles. After the peak of contraction, the sample dilates continuously. A maximum shear stress is obtained around 0.65% of macroscopic axial deformation.
2.2 Macroscopic shear banding

Many experiments and theoretical works have been conducted in the past in order to describe and understand the onset of macroscopic strain localization within shear bands in geomaterials. Important insights into the mechanics of macroscopic localization were obtained from the continuum analysis of its inception as a bifurcation in the constitutive law [10]. In discrete materials such as soils, the localization of deformation into thin zones of intense shearing is a phenomenon commonly observed [11-14]. It is also assumed that, in the early stages of deformation, homogeneous deformation is observed, while patterns of strain localization appear at some point throughout the test, generally at the peak load or slightly before [11]. It has been reported that these shear bands can form and disappear as deformation proceeds after the peak load [11].

These features are qualitatively observed within our DEM simulations. Figure 2 shows the incremental shear strain fields (computed using equation 2, see section 3) obtained at different stages of the loading by integrating the grains displacements over large deformation windows equal to $\delta \varepsilon_{\text{large}} = 2.4 \times 10^{-3}$. We can see that, while heterogeneous, the incremental shear strain field at the beginning of the test (figure 2.1) does not show any clear macroscopic structure. However, as loading goes on, a macroscopic localization materialized by a shear band that spans the entire sample can be distinguished slightly before the peak load (Figure 2.2). Then, these structures essentially perpetuate in time (figure 2.3).

Figure 2: Incremental shear deformation fields from the beginning of the test to the end of the peak load. The shear strain fields are computed by considering deformation windows, of size $\delta \varepsilon_{\text{large}} = 2.4 \times 10^{-3}$, materialized on figure 1 (corresponding numbers).
However, by looking more precisely on the incremental strain field, i.e. by considering smaller deformation windows to compute the grains displacements, things become more complex. Associated to the disordered spatial structure of the force network of the initial static granular material [15], intermittent strain heterogeneities emerge from the beginning of the test: patches of variables sizes of intense deformation appear through specific zones, they brutally disappear and the strain field switches to different patterns. Consequently, the mechanical behavior of granular media qualitatively looks highly heterogeneous and intermittent. This intermittency and heterogeneity of the strain field is the key point we aim to quantify in this paper, in order to answer to the following questions: Is this emergence of intermittency and heterogeneity associated to specific scaling laws? Can these processes be connected to final shear banding we observe on figure 2, as a result of the coalescence and interaction of structured localized zones?

To answer to these fundamental questions, we perform a coarse graining analysis on the strain rate field.

3 **COARSE GRAINING ANALYSIS**

Incremental strain are computed over a broad range of spatial scales at different stages of macroscopic deformation from a coarse graining analysis similar to that of Marsan et al. [16]. The configurations are saved for each simulation with a constant deformation interval $\delta \varepsilon_w$ chosen to be equal to $5 \times 10^{-6}$. This choice for $\delta \varepsilon_w$ is justified in section 4.3. The increments $(u_i, v_i)$ of displacements of each particle $i$ are computed from the difference in the particle positions $(x_i, y_i)$ between two successive configurations. Then, a mesh triangulation is performed on the grains centers, and the spatial derivatives $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$, $\frac{\partial v}{\partial x}$ and $\frac{\partial v}{\partial y}$ of the incremental displacements associated to each element of the mesh are computed following a contour integral.

In the following, we focus on two invariants of the incremental strain tensor:
- the divergence
\[
\delta \varepsilon_v = \delta \varepsilon_1 + \delta \varepsilon_2 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}
\] (1)
- the shear
\[
\delta \gamma = \delta \varepsilon_1 - \delta \varepsilon_2 = \sqrt{\left(\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)^2}
\] (2)

where $\delta \varepsilon_1$ and $\delta \varepsilon_2$ are the principal components of the incremental strain tensor.

The scaling properties of the incremental divergence and shear fields are then explored from a coarse graining analysis [6,16].

First, deformation at the micro scale, i.e. the mesh scale, is computed. Then, at larger spatial scales, deformation is obtained by splitting the sample into square cells of size ranging from the micro scale to the macro scale (the simulation box). Consider a square cell of width $W$ at a certain location within the sample. We find all the element centers of the mesh that lie inside the box and compute the average spatial derivatives $\frac{\partial u}{\partial x}$, over all the corresponding elements,
where the contribution of each element is weighted by its area. From these gradients, thus averaged at the scale $W$, we compute the incremental strain invariants $\delta \varepsilon_v$ and $\delta \gamma$ following (1) and (2). Assuming scaling isotropy, we define the effective spatial scale $L$ of the cell as the square root of the area covered by the elements (which is close but not exactly equal to $W$). This procedure is repeated for all the other cells of the same width $W$ that cover the sample (no overlap is considered here). Average values $\langle | \delta \varepsilon_v | \rangle$ and $\langle \delta \gamma \rangle$ are computed by averaging the incremental divergent strain modulus $| \delta \varepsilon_v |$ and the incremental shear strain $\delta \gamma$ over all the cells of the same width. $W$ is logarithmically binned starting from $W_{macro}$ i.e. $W$ is iteratively equal to $W_{macro}$, $W_{macro}/2$, $W_{macro}/4$, etc... (Figure 3).

![Figure 3: Illustration of the coarse graining method on a sample of 2500 grains. The green arrows show the displacement vector for each grain between the two successive configurations taken near the peak load. The red boxes show the areas considered to compute the incremental strains at scales ranging from macro to micro scale.](image)
4 RESULTS

In the following, all the results are averaged over coarse graining analyses conducted on 50 simulations of 10000 grains. Similar results were obtained with simulations of 45000 grain. From one simulation to another, the only changing sample property is the initial random organization of the grains in space, inducing changes within the force network disorder.

4.1 Contractancy

Figure 4 plots the average of the incremental divergent strain modulus \(<|\delta \varepsilon_v|>| as a function of scale \(L\) in the early stages of biaxial testing, up to dilatancy (Figure 4). At the early stages of deformation (\(\varepsilon_1 = 1.1 \times 10^{-3}\)), black curve on Figure 4(b), \(<|\delta \varepsilon_v|>| does not vary with \(L\), which means that the incremental divergent deformation is homogeneously scattered throughout the sample. As macroscopic deformation proceeds, a decrease of \(<|\delta \varepsilon_v|>| with \(L\) is observed at small scales while, for \(L\)-values larger than a crossover scale denoted \(L_v^*\), a plateau is observed. This means that, for \(L < L_v^*\), the incremental divergent deformation is heterogeneous while homogeneity can only be assumed for \(L >> L_v^*\). Finally, at the point corresponding to the maximum of contraction (i.e. the onset of macroscopic dilation), a power law scaling over the entire range of scales is observed on \(<|\delta \varepsilon_v|>|: the divergent incremental deformation is at that point highly heterogeneous, from the grain scale to the macroscopic scale, and no characteristic size appears.

These results suggest a progressive structuring of the divergence rate field as approaching the peak of contraction, where the crossover scale \(L^*\), interpreted here as a correlation length [6], diverges. To test this hypothesis, we define a control parameter \(\Delta_v\) as follows:

\[
\Delta_v = \frac{\varepsilon_{1v} - \varepsilon_1}{\varepsilon_{1v}}
\]
where $\varepsilon_1^{cv} = 2.9 \times 10^{-3}$ is the value of axial deformation $\varepsilon_1$ at the peak of contraction. Thus, $\Delta v$ is equal to 0 at $\varepsilon_1 = \varepsilon_1^{cv}$, and the mean incremental divergent strain modulus can be expressed as

$$<|\delta \varepsilon_v|>(L, \Delta v) \sim L^{-\rho v} H_v \left( \frac{L}{L_v^*} \right) \tag{4}$$

where $H_v$ describes the crossover: it is thus constrained by $H_v \left( \frac{L}{L_v^*} \right) \sim \text{const}$ for $L \ll L_v^*$ and $H_v \left( \frac{L}{L_v^*} \right) \sim L^{\rho v}$ for $L \gg L_v^*$. 

We further hypothesize that $L_v^*$ diverges as approaching $\varepsilon_1^{cv}$ as $L_v^* \sim A^{-\nu_v}$, and we estimate the exponent values from a data collapse analysis (Figure 5).

![Figure 5: Data collapse analysis of the average divergence rate. The values used for the exponents are $\rho_v = 0.55 \pm 0.05$ and $\nu_v = 1.5 \pm 0.1$.](image)

$\rho_v = 0.55 \pm 0.05$ and $\nu_v = 1.5 \pm 0.1$ allow the best collapse.

We tested the significance of this observation by randomly reshuffling the spatial derivatives of the incremental displacements in space. Doing this, the coarse graining analysis shows no power law trend. Hence, the observed power law scaling of $<|\delta \varepsilon_v|>$ with $L$ at the peak of contraction is the result of the spatial correlations present in the divergent deformation field and can be related to the spatial structure of the deformation field. The correlation length $L_v^*$ is small at the onset of macroscopic deformation, and represents in this case the size of a representative elementary “volume” (REV). On the other hand, the power law divergence of the correlation length $L_v^*$ at $\varepsilon_1 = \varepsilon_1^{cv}$ leads us to conclude that the peak of contraction plays the role of a critical point with respect to the divergent deformation field in granular materials. On the contrary, at that stage, no scaling is observed for the incremental shear deformation field $\langle \delta \gamma \rangle$. 

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Florent Gimbert, Gael Combe, David Amitrano and Jérôme Weiss
4.2 Shear banding

In order to see if a similar “critical-like” behavior can be associated to macroscopic shear faulting and/or the onset of macroscopic softening, we performed a coarse graining analysis on the incremental shear deformation $<\delta \gamma>$. Strain configurations are selected in this case with respect to the loading curve $\tau$ versus $\varepsilon_1$ (Figure 6(a)), where $\tau = (\sigma_1 - \sigma_3)/\sigma_3$ is the deviatoric stress. Looking at $<\delta \gamma>$ versus $L$ on Figure 6(c), a similar behavior with the one presented in the previous section on the divergent strain field is observed: a rather homogeneous incremental shear strain field (i.e. a small associated correlation length) is observed in the early stages of deformation, and a power law scaling is building up as $\varepsilon_1$ increases.

The power law decrease of $<\delta \gamma>$ with $L$ at small scales shows an exponent $\rho_s$ equal to 0.3. However, unlike what was observed for the incremental divergent deformation in the preceding section, from $\varepsilon_1^{sat} = 4.1 \times 10^{-3}$, the correlation length $L_{s}^{sat}$ seems to saturate at a value $L_{s}^{sat} = 30D_{max}$. In other words, power law scaling never develops over the entire scale range in the present case. We checked that $L_{s}^{sat}$ does not depend on the size of the system considered, i.e. does not result from a finite size effect.

Nevertheless, we verified that a scaling similar to equation (4) well describes the results of figure 6b and the corresponding increase of $L_{s}^{sat}$, up to the limiting value $L_{s}^{sat}$. To do so, we define, following equation (3), a second control parameter $\Delta_s$ equal to 0 at an axial deformation $\varepsilon_1 = \varepsilon_1^{cs}$, and express the average incremental shear strain as:

$$<\delta \gamma> (L, \Delta_s) \sim L^{-\rho_s} H_s \left( \frac{L}{L_{s}^{sat}} \right)$$

where $H_s$ describes the crossover as in previous section. At this stage, $\varepsilon_1^{cs}$ is unknown but is necessarily larger than $\varepsilon_1^{sat}$. 
We then hypothesize that $L_s^*$ grows as $L_s^* \sim \Delta_s^{-\nu_s}$, and we estimate the exponent values as well as the axial strain $\varepsilon_1^{cs}$ from a data collapse analysis (Figure 6).

\[ \varepsilon_1^{cs} = 4.2 \times 10^{-3}, \ \rho_s = 0.3 \pm 0.05 \text{ and } \nu_s = 2.0 \pm 0.2 \text{ allow the best collapse.} \]

This collapse works well for $\Delta_s \geq 0.15$ i.e. for values of axial deformation $\varepsilon_1$ lower than $3.6 \times 10^{-3}$, providing that the choice of $\varepsilon_1^{cs} = 4.2 \times 10^{-3}$ is convenient. However, when axial deformation proceeds further towards $\varepsilon_1^{cs}$ (i.e. $\varepsilon_1 > 3.6 \times 10^{-3}$), a deviation from the scaling form (5) is observed (black dashed circles on Figure 6), as the result of the saturation of the correlation length. This saturation indicates that the divergence is not complete.

Consequently, the shear deformation rate field seems to organize with respect to a specific level of applied strain $\varepsilon_1^{cs} = 4.2 \times 10^{-3}$, although this evolution is stopped before to spread over the full range of spatial scales, near $\varepsilon_1 = 3.6 \times 10^{-3}$.

It is interesting to note that this axial strain $\varepsilon_1^{cs} = 4.2 \times 10^{-3}$ corresponds to a deformation stage slightly before the peak load, corresponding to the point at which the formation of a macroscopic shear band is qualitatively reported in experiments [11] and also in our DEM model (Figure 2), as the shear strain field #2 plotted on figure 2, computed over an axial strain window of $\delta \varepsilon_{large} = 2.4 \times 10^{-3}$, exactly starts at $\varepsilon_1^{cs} = 4.2 \times 10^{-3}$. When calculated over a much smaller strain window of $5 \times 10^{-6}$, the incremental shear strain field at $\varepsilon_1^{cs}$ (figure 6c) shows strain clusters, however not organized into a macroscopic shear band spanning the entire sample. Unlike the shear bands of figure 2, these strain clusters do not perpetuate and are instead highly intermittent (not shown). Therefore, the structuration of the shear strain seems to be dependent on the size of the strain window considered.
4.3 Strain window size dependency

The calculations shown in section 4.2 were performed using a deformation window $\delta \varepsilon_w$ of $5 \times 10^{-6}$ between two successive configurations. While considering larger deformation window sizes does not affect the dependence of $\langle |\delta \varepsilon_v| \rangle$ with $L$ (similar results than the one shown in section 4.1 are reported), this is not the case for $\langle \delta y \rangle$. Because highly intermittent in time in the vicinity of the peak load, the scaling properties of the incremental shear field are largely affected by the deformation window size, i.e. the value of $\delta \varepsilon_w$ considered to compute the grains displacements. Figure 7 plots the results of the coarse graining analysis performed around $\varepsilon^{cs} = 4.2 \times 10^{-3}$ for several values of $\delta \varepsilon_w$, ranging from $5 \times 10^{-6}$ to $2.4 \times 10^{-3}$.

![Figure 7: Influence of the deformation window size $\delta \varepsilon_w$ on the scaling properties of the deformation field at $\varepsilon^{cs} = 4.2 \times 10^{-3}$. Colored continuous lines are computed by considering deformation windows centered at $\varepsilon^{cs}$. The black dashed line results from a coarse graining analysis conducted on the incremental shear strain field #2 of Figure 2, obtained with a simulation of 45000 particles.](image)

The departure from power law behavior at large spatial scales $L$ as $\delta \varepsilon_w$ increases is obvious on this plot. It has been checked that the multi-scale properties of the shear rate deformation field are not affected when considering values of $\delta \varepsilon_w$ five times smaller than $5 \times 10^{-6}$. This means that, at $\varepsilon^{cs} = 4.2 \times 10^{-3}$ and for small deformation window sizes (inferior to $5 \times 10^{-5}$), the shear strain field is characterized by large correlation length values, up to $30D_{\text{max}}$. By opposition, small correlation lengths of about $3D_{\text{max}}$ clearly appear when considering large deformation window sizes, i.e. greater than $2 \times 10^{-5}$. These small correlation lengths observed at large deformation windows seem to be robust, since the cross-over remains approximately the same for values of $\delta \varepsilon_w$ varying of 2 orders of magnitudes, from $5 \times 10^{-3}$ to $2.4 \times 10^{-3}$.

Thus, two distinct behaviors can be outlined:

- Large correlation lengths are reported at small strain window sizes. This point out the fact that elastic interactions between particles allow the system to communicate via long range interactions. The associated spatial deformation field pattern is materialized by patches of intense shearing, highly intermittent in space and time.
• Small correlation lengths are reported at large strain window sizes. This means that the intermittent character of the shear deformation field associated to the development of self affine structures observed at small strain window sizes within the deformation field gives rise to the observation of a macroscopic shear band at large enough strain window sizes. The correlation length given by the coarse graining analysis is associated to the width of the macroscopic shear band, here equal to $3D_{\text{max}}$.

5. CONCLUSION

We have shown that, during compressive loading, spatial correlations associated to the coalescence and interaction of structured localized zones take place within the deformation field of frictional granular materials. The associated correlation length can be extracted from a coarse graining analysis. Specific scaling properties of the divergent and shear strain field, which behave separately, are associated to macroscopic evidences:

• The divergence of the correlation length associated to the incremental divergent strain field modulus as approaching the onset of macroscopic dilation is reported. This means that the peak of contraction, located at $\varepsilon_1^{\text{cv}} = 2.95 \times 10^{-3}$, plays the role of a critical point with respect to the divergent deformation field.

• The increase of the correlation length within the incremental shear strain field is reported until $\varepsilon_1^{\text{cs}} = 4.2 \times 10^{-3}$ is reached, where a remaining saturation is observed at large scales on the power law scaling. We have shown that the shear deformation field organizes itself with respect to a specific level of applied strain $\varepsilon_1^{\text{cs}} = 4.2 \times 10^{-3}$, located slightly before the peak load. We argue that this point corresponds to the onset of macroscopic shear banding.

Finally, because highly intermittent in time and space, the shear strain field shows scaling properties that are largely controlled by the strain window size considered. Large spatial correlations are observed at small strain windows, while small spatial correlations, equal to the width of the macroscopic shear band when looking after $\varepsilon_1^{\text{cs}} = 4.2 \times 10^{-3}$, are observed at large strain windows.

A remaining question is how such intermittency observed at very small time scales within the deformation field, meaning that the deformation field loses its memory rapidly, leads to the development of perennial structures materialized by a macroscopic shear band at large time scale.

REFERENCES


Mesoscopic scale modeling of concrete under triaxial loading using X-ray tomographic images

C. POINARD*, E. PIOTROWSKA*, P. MARIN*, Y. MALECOT* AND L. DAUDEVILLE*

* UJF-Grenoble 1, Grenoble-INP, CNRS UMR 5521, 3SRLab, Grenoble F-38041, France.
e-mail: cedric.poinard@hmg.inpg.fr

Key words: Concrete behaviour, Compressive triaxial tests, Mesoscopic modeling, Segmentation, X-ray tomography

Abstract. This paper focuses on the discrete modeling of triaxial behaviour of concrete. The originality of this work comes from two points. The first one concerns the predictive feature of the model developed for simulating the response of concrete specimens; the behaviour of mortar, rock, and their interaction being identified a priori or by means of experimental tests on the mortar and the rock. The second originality relates to the construction method of the discrete element assembly based on the 3D segmentation of tomographic images. Such a method allows modeling of concrete at the mesoscopic scale with an internal structure similar to the one of the concrete tested experimentally. The comparisons between numerical and experimental results show the model is capable to reproduce the triaxial behavior of concrete for confining pressure varying from 0 to 650 MPa.

1 INTRODUCTION

Concrete is a complex material that is a subject of numerous research studies. One of them is related to its behavior under violent explosion or ballistic impact. For such solicitations, concrete undergoes severe triaxial loading [1,2]. In order to improve this research field, several authors characterized the triaxial behavior of concrete by performing quasi-static tests [3,4], in particular Gabet et al. [5,6] who were the first ones to use a very high capacity triaxial press to analyze the triaxial behaviour of concrete under very high confinement. All of these studies led to the same conclusions, the confinement improves the strength of concrete and influences the failure pattern. Vu et al. also showed that the E/C ratio, governing the uniaxial behavior, has no influence under high confining pressure whereas the saturation ratio becomes predominant [7,8].

In order to improve the understanding of mechanisms leading to the failure of concrete under triaxial loading, Poinard et al combined the X-ray tomography with other classical observation methods [9,10]. Even though X-ray tomography allows to reveal the modification of damage mechanisms with increasing confining pressure, they still remain difficult to characterize, particularly under high confinement. One of the main problems is the impossibility to access the internal structure of concrete during loading.

In order to face such difficulties, the multiphase modeling, that takes into account the
heterogeneities of the material, can be an interesting tool since it enables accessing the internal structure of concrete at any time of the test. Recently, mesoscopic models have been developed in order to differentiate the elements corresponding to the mortar, to the biggest aggregates [11,12] and possibly to the interface between both constituents [13]. These models are capable to reproduce concrete behavior for a more or less important range of experimental tests [14].

For the purpose of this study, a mesoscopic modeling using the principles of lattice models [15] and discrete element method [16] are used to reproduce the concrete behavior under severe triaxial loading. The originality of this approach comes from the predictive feature of the developed model on the one hand; the behavior of mortar, of aggregates and their interaction being identified a priori or from experimental tests realized on the mortar and the rock. On the other hand, the numerical sample construction relies on the 3D segmentation of tomographic images of the R30A7 concrete, material extensively studied by Gabet et al. [5,6], Vu et al. [7,8], and Malecot et al. [17]. Such a construction method enables to obtain a numerical specimen with an internal structure similar to the real one.

The first part of this paper will cover the construction method of the numerical specimen. We will see the different steps allowing to obtain an assembly of spheres that represents the real mesostructure of the R30A7 concrete. Subsequently, the features of the model will be presented, i.e. the different types of interactions and the laws governing their behavior. Since concrete is modeled as the large aggregates surrounded by the mortar, the third part will interest in the macroscopic modeling of this two constituents in order to know the parameters associated to the interactions mortar-mortar and aggregate-aggregate. Finally, after an a priori identification of the parameters associated to the aggregate-mortar interactions, we will present the ability of the model to reproduce the triaxial behavior of concrete.

2 CONSTRUCTION OF THE NUMERICAL CONCRETE SPECIMEN

The numerical concrete specimen corresponds to a cubic and heterogeneous assembly of spheres that interact each other. The distribution of material throughout spheres of different sizes enables to work easily with contact interactions that mainly occur after failure of cohesive interactions. This assembly is heterogeneous in the meaning that the spheres represent materials of two different natures: rock and mortar. In addition, the macropores are taken into account and represented by the absence of spheres. The construction of this sample is based on a three-step procedure: the segmentation of images representing the concrete mesostructure, the assemblage of spheres and the identification of the nature of spheres.

2.1 Segmentation of images representing the R30A7 concrete mesostructure

Segmentation is a process that consists in partitioning an image into multiple segments (set of pixels) sharing certain characteristics. For the purpose of this study, two segmentation methods have been developed and then applied to X-ray tomographic images (slices) of R30A7 concrete. The scan parameters were chosen to well represent the mesostructure on the slices. Consequently, the concrete can be seen as a triphasic material constituted of mortar, aggregates and macropores (entrapped porosity). Figure 1 (a) exhibits one of the slices of a cylindrical specimen: the lowest gray levels (black) represent the pores, the highest ones the
aggregates and those intermediate the mortar. Thus, the aim of these two segmentation methods is to isolate the mortar and aggregates in order to create a new concrete specimen in which the meso-constituents are well localized.

**Entrapped porosity segmentation**

The entrapped porosity segmentation is detailed in the article of Poinard et al. [9]. The image processing used, called thresholding, consists in transforming a gray level image into a binary image through a threshold gray level. In our case, since there is an uncertainty on the threshold gray level, it has been identified in order to obtain a value of porosity corresponding to the entrapped porosity measured experimentally. Figure 1 (b) presents the result of the thresholding step. In order to have an image constituted only of pores, it is then required to remove the background (Figure 1(c)). This porosity segmentation can be applied slice by slice or to a volume as well.

![Figure 1: Step of porosity segmentation](image)

- (a) concrete slice obtained by Rx tomography
- (b) after threshold processing
- (c) after removing the background

**Aggregates segmentation**

The segmentation of aggregates is more complicated to realize since the grey levels of both aggregates and mortar are partially mixed up. Nevertheless, on the slices representing the R30A7 concrete mesostructure, these two constituents exhibit a different feature, which is the homogeneity of the gray levels. Thus, the aggregates segmentation method is based on a “standard deviation” filter that enables to differentiate the gray levels of mortar from the ones of aggregates. Since the segmentation is applied to a set of slices, and so a volume, the standard deviation filter used is cubic. Its size has been chosen in order to obtain the best segmentation as possible. Figure 2 (a) exhibits one of the slice of the cylindrical specimen before and after application of the standard deviation filter. It clearly appears, on both treated slice and associated gray level histogram, that the aggregates are now represented by gray levels higher than the ones of mortar (two peaks on the gray level histogram), even if there is a small overlap. After the application of the standard deviation filter, a thresholding step allows to isolate the voxels corresponding to the aggregates. To do that, the threshold grey level is set to the minimal value between both peaks. Finally, simple modifications such as removing porosity are applied to obtain images representing only the large aggregates. Figure 2(b) exhibits a slice once the aggregates segmentation is done.
Once the aggregates and porosity segmentations are done, they are combined to rebuild the concrete volume (Figure 3).

2.2 The spheres assembly construction

The spheres assembly construction is independent of what has been done in the previous section. This step starts by meshing a cube with tetrahedrons and continues by the application of an algorithm allowing to obtain an assembly of spheres. This algorithm described in Jerrier et al. [19], consists in filling each tetrahedron with spheres in the following way:
- at the center of each edge
- on the nodes
Once the aggregates and porosity segmentations are done, they are combined to rebuild the concrete volume (Figure 3).

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- at the center of each edge
- on the nodes
- on the triangular faces
- at the center of tetrahedron
- and in the void space

The interest of such a process is to provide an isotropic assembly of different size spheres assuring no orientation preference during failure. A cubic assembly of 9449 spheres was made for the purpose of this study.

2.3 Identification of the nature of spheres

The identification of the spheres nature consists in overlaying both cubes, the one segmented (section 2.1) and the one composed of spheres (section 2.2). The material is then assigned to each sphere depending on its position in the segmented cube. In addition, the spheres corresponding to the pores are removed out of the assembly what reduces the total number of spheres from 9449 to 9113. The Figure 4 exhibits the mesostructure of R30A7 concrete in both segmented cube and numerical specimen. For the assembly of spheres, a visualization by Voronoï cells has been chosen with a representation of pores.

![Figure 4: Mesostructure of a R30A7 concrete:](image)

(a) in the segmented cube, the black corresponding to the pores, the white to the aggregates and the grey to the mortar
(b) in the assembly of 9449 voronoï cells, the green corresponds to the pores, the red to the aggregates and the blue to the mortar

Table 1 presents the volume percentages of the different materials in a REV of concrete, in the segmented cube and in the numerical concrete sample of 9113 spheres. The proportions of the R30A7 meso-constituents are well preserved in the segmented cube and in the assembly of spheres. Nevertheless, it must be mentioned that even if the porosity percentages are very close, the number of pores in the numerical specimen is strongly reduced.

<table>
<thead>
<tr>
<th>Material</th>
<th>REV of concrete</th>
<th>Segmented cubic</th>
<th>Assembly of 9113 spheres</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mortar (%)</td>
<td>59,5</td>
<td>63,4</td>
<td>62,8</td>
</tr>
<tr>
<td>Aggregates (%)</td>
<td>37</td>
<td>33,2</td>
<td>33,7</td>
</tr>
<tr>
<td>Entrapped porosity (%)</td>
<td>3,5</td>
<td>3,4</td>
<td>3,5</td>
</tr>
</tbody>
</table>
3 THE DISCRETE MODEL

The particularity of the proposed discrete method relies on the use of both the principle of the lattice model, in which the specimen is represented by a beam network, and the principle of the classical discrete element method, in which the material is represented by a collection of rigid spheres interacting by contacts. The combination of these two models enables reproducing the triaxial behaviour of concrete up to very high confining pressures.

3.1 The interactions

Two kinds of interaction are distinguished in the model: the cohesive interactions (beam network) and the contacts. The cohesive interactions govern an important part of concrete behavior, particularly in the absence of the confinement. They are created at the beginning of the simulation, before any displacement, if the initial distance $D_{\text{init}}$ between two spheres is sufficiently small \( (1) \). The interaction radius $\lambda_{\text{coh}}$ is defined in order to obtain an average of 12 cohesive interactions by sphere, what assures a good reproducibility of the elastic features (Hentz et al. [18] and Rousseau et al. [20,21]). The cohesive interactions may break during simulation.

$$\lambda_{\text{coh}}(R_a + R_b) \geq D_{\text{init}} \quad (1)$$

with $R_a$, $R_b$, $D_{\text{init}}$ defined in Figure 5.

![Figure 5: Features of an interaction](image)

The contact interactions are required to reproduce the behavior of concrete under high confinement. They occur during the simulation when two spheres, not linked by a cohesive interaction, get significantly closer. Actually, most of the contacts appear in place of cohesive interactions broken in traction, when the two spheres come back to the initial distance.

3.2 The behavior laws

This section presents briefly the behavior laws introduced at the interaction scale. The interaction force $F$ representing the action of element $a$ on element $b$ (Figure 5) can be decomposed into a normal force $F_N$ and a shear force $F_S$. Figure 6 presents the relation between the normal force and the distance $D$ between the centers of the two spheres.
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The compressive behavior of interactions is similar to the one observed at the macroscopic scale for cement matrix materials during hydrostatic compression tests. It starts by a linear elastic phase governed by the stiffness $K_N$ (2), what is followed by a compaction phase controlled by the non-linear stiffness $K_{N2}$ (3). After the consolidation point, the behavior is linear elastic with the stiffness $K_{N3} > K_N$ (4).

$$F_N = (D_{\text{init}} - D)K_N$$ (2)

$$F_N = (D_{\text{init}} - D_{\text{el}})K_N + (D_{\text{el}} - D)K_{N2}$$ (3)

$$F_N = (D_{\text{init}} - D_{\text{el}})K_N + (D_{\text{el}} - D_{\text{cons}})K_{N2} + (D_{\text{cons}} - D)K_{N3}$$ (4)

The tensile behavior of the cohesive interactions is governed by an elastic brittle law with damage (5). The failure appears when the normal force exceeds the tensile strength and is more or less brittle depending on the value of the softening parameter $\zeta$.

$$F_N = (D - D_{\text{max}})\frac{K_N}{\zeta}$$ (5)

The tangential behavior is governed by the tangential stiffness $K_S$ (Figure 5) through the modified mohr coulomb law (Figure 7). The limitation of the tangential force facilitates the tangential sliding and so the arrival of the failure of interactions. It must be noted that to take into account the elements size variation, the surface $S_{\text{int}}$, defined by $\min(\pi R_a^2, \pi R_b^2)$ (Figure 5) is used.

Figure 6: Normal behavior law of cohesive and contact interactions

Figure 7: Tangential behavior law of cohesive and contact interactions

The compressive behavior of interactions is similar to the one observed at the macroscopic scale for cement matrix materials during hydrostatic compression tests. It starts by a linear elastic phase governed by the stiffness $K_N$ (2), what is followed by a compaction phase controlled by the non-linear stiffness $K_{N2}$ (3). After the consolidation point, the behavior is linear elastic with the stiffness $K_{N3} > K_N$ (4).
3.3 Strategy for modeling the concrete behavior at the mesoscopic scale

The behavior laws presented in the previous part are governed by numerous parameters that need to be identified. Since concrete is modeled as a heterogeneous material, these parameters depend on the nature of the interaction: mortar-mortar, mortar-aggregate, etc. The strategy consists of modeling mortar and rock as homogeneous materials in order to determine the parameters of interactions mortar-mortar and aggregate-aggregate. The following steps of the trial and error identification procedure are performed:

- Simple compression tests to identify the normal stiffness $K_N$ and the tangential stiffness $K_S$ that reproduce the elastic features $E$, $\nu$ of the material.
- Simple compression tests and tensile tests to identify $T$, $\zeta$ and $C_0$ that reproduce as much as possible the pre and post peak behavior of the material.
- Hydrostatic compression tests to identify the nonlinear stiffness $K_{N2}$
- Triaxial compression tests at different confining pressures to identify the parameters $C_1$, $\phi_i$ and $\phi_c$.

For the aggregate-mortar interaction, since we don’t have any experimental tests, an a priori identification of the parameters is performed, what will be detailed in section 5.1.

4. MACROSCOPIC MODELING OF THE CONSTITUENTS EXISTING IN THE MESOSTUCTURE OF THE R30A7 CONCRETE

4.1 Mortar

This section shows the capability of the model to simulate the behavior of mortar characterized experimentally by Dupray et al. [12]. Simple compression test presented in Figure 8 shows very good reproducibility of experimental results in terms of elastic parameters, limit states (stress peak and contractancy-dilantancy transition) and post peak behavior.
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Figure 9 interests in the triaxial compression tests at different levels of confinement. The numerical sample reproduces in a remarkable way the behavior of mortar: not only are the contractancy-dilatancy transition reproduced, but also the shape of curves. The increase in ductility with the confining pressure found experimentally, is also observed numerically. The stiffness of the numerical specimen is significantly lower than the one of the mortar at the early stages of deviatoric loading at high confinement. This difference can be largely explained by the creep existing at the beginning of the deviatoric part of the experimental test and not taken into account in the simulations.

4.2 Rock

The behavior of the quartzite sandstone existing in the form of aggregates in the R30A7 concrete has been characterized through experimental tests: uniaxial compression, triaxial compression at 50 MPa, hydrostatic compression and Brazilian test. Figure 10 shows the comparison between numerical and experimental results for three different compressive tests. We can observe that the elastic features, the stress peaks and the post peak behaviors are well reproduced by the model. Nevertheless it must be mentioned that it is not possible to
satisfactorily reproduce the value of tensile strength determined from the Brazilian test (23 MPa) at the same time. It remains overestimated and equal to 40 MPa.

Figure 10: Behavior of a quartzite sandstone
(a) uniaxial compression
(b) triaxial compression at 50 MPa
(c) hydrostatic compression

5. MESOSCOPIC MODELING OF R30A7 CONCRETE TRIAXIAL BEHAVIOR

The simulations presented in section 4 allowed to identify the parameters of mortar-mortar interaction and aggregate-aggregate interaction. Therefore, the parameters of two other types of interaction must be determined: mortar-aggregate and aggregate-aggregate (two different aggregates). The parameters governing aggregate-aggregate interaction were chosen equal to those of mortar-aggregate interaction what is justified by their low percentage and the fact that two aggregates are inevitably separated by a layer of mortar.

5.1 Parameters identification of the aggregate-mortar interaction

The parameters of the aggregate-mortar interaction are identified in an a priori manner due to the lack of experimental results. For the microscopic stiffnesses $K_N$ and $K_S$ governing the elastic behavior, the mean of the stiffnesses of rock and mortar are used. This choice is explained by the fact that the stiffness of an aggregate-mortar interaction can be seen as two stiffnesses in series, the one of mortar and the one of rock. Equation 6 presents the computation of the normal stiffness $K_N$ defined by $K_{N\text{,interface}}$ for the aggregate-mortar interaction.

$$K_{N\text{,interface}} = \frac{2(K_{N\text{,mortier}} K_{N\text{,granulat}})}{K_{N\text{,mortier}} + K_{N\text{,granulat}}}$$

Some authors showed that there exist the “Interfacial Transition Zone” between aggregates and cement paste that exhibits poor mechanical properties [22]. In order to take into account the weakness of this zone, the strength properties $(T,C_0)$ are chosen as mortar properties divided by the degradation coefficient, which is calibrated to reproduce the uniaxial strength. The other parameters of the aggregate-mortar interaction were chosen in order to obtain the best reproduction of the triaxial behavior of R30A7 concrete.

5.2 Behavior of the numerical concrete

Figures 11 et 12 shows the ability of the numerical concrete, defined as an heterogeneous
assembly of spheres, to simulate the behavior of R30A7 concrete under compression tests more or less confined. The curves presented in Figure 11 show that the numerical concrete behaves in a quasi-identical manner with the real concrete during an uniaxial compressive test. The only difference concerns the post peak phase when the behavior is slightly less brittle numerically than experimentally.

Figure 11: Uniaxial behavior of concrete
(a) axial and transverse behavior
(b) volumetric behavior

Figure 12 shows that the model is also efficient when simulating the triaxial compression tests at confinement ranging from 50 to 650 MPa. Indeed, the limit states (stress peak or plateau and contractancy-dilatancy transition) of the numerical and real concrete occur at comparable stress and strain levels, particularly for the low confinement. At the 650 MPa of confinement, the model slightly underestimates concrete strength.

Figure 12: Triaxial behavior of concrete
(a) axial and transverse behavior
(b) volumetric behavior

6 CONCLUSIONS

A discrete model was used to reproduce the triaxial behavior of concrete. The model is realized at the mesoscopic scale, what means that the features of the three concrete mesostructure constituents: aggregates, mortar, pores, and their interaction are taken into account. In addition, in order to perform simulations on a numerical specimen similar to the
real concrete, an original method of mesh conception based on the segmentation of
tomographic images has been developed.

The comparison between behavior curves coming from simulations and experimental tests
showed the model is capable to reproduce the concrete response under triaxial loading more
or less confined. Nevertheless, a macroscopic modeling, that is more simple, would be as
much efficient. Besides, it was used to reproduce the behavior of mortar.

This mesoscopic modeling method is thus developed in order to improve the understanding
of mechanisms leading to the failure of concrete subjected to high triaxial loadings, on one
hand. Besides, work on the damage visualization is being developed in order to assess the
model ability to reproduce the mechanisms observed experimentally. On the other hand, such
a model, if it is enough consistent, might progressively replace the experimental tests to study
the influence of the concrete mesostructure (aggregates size, aggregates volume/mortar
volume, macroporosity, etc.) on the triaxial behavior.

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UNIVERSALITY CLASS OF THE FRAGMENTATION OF PLASTIC MATERIALS

F. KUN*, G. TIMÁR*, J. BLÖMER†, AND H. J. HERRMANN‡

*Department of Theoretical Physics, University of Debrecen
P. O. Box: 5, H-4010 Debrecen, Hungary
feri@dtp.atomki.hu

†Spezialwerkstoffe, Fraunhofer UMSICHT, Osterfelder Str. 3, 46047 Oberhausen, Germany

‡Computational Physics IfB, HIF, ETH, Hönggerberg, 8093 Zürich, Switzerland

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Abstract. We carry out an experimental and theoretical study of the fragmentation of polymeric materials by impacting polypropylene (PP) particles of spherical shape against a hard wall. Our experiments revealed that the mass distribution of fragments has a power law behavior with an exponent close to 1.2, which is significantly different from the known exponents of three-dimensional bulk materials. To understand the fragmentation of plastic materials we developed a three-dimensional discrete element model where the sample is represented as a random packing of spherical particles connected by elastic beams. The model reproduces both the large permanent deformation of the polymer during impact, and the novel value of the mass distribution exponent. Computer simulations revealed that the dominance of shear in the crack formation and the healing of compressed crack surfaces are the key features which give rise to the emergence of the novel universality class of fragmentation phenomena.

1 INTRODUCTION

Fragmentation of heterogeneous materials is a very complex scientific problem with an enormous technological importance [1, 2]. From the usage of explosives in mining through the comminution of minerals to the liberation of grains in particle composites fragmentation processes play a crucial role which calls for a thorough understanding. During the last decade research efforts have been concentrated on the breakup of heterogeneous brittle materials which is by now fairly understood [1, 2, 3, 4, 5, 6, 7, 8]. Experimental and theoretical investigations have revealed that the energy imparted to the solid has to surpass a threshold value (critical energy) to achieve complete breakup [4, 5, 6]. In this fragmented state the mass (size) distribution of pieces follows a power law functional form
with universal exponent depending mainly on the effective dimensionality of the system
[1, 3, 4, 5, 6, 7, 8]. The branching-merging scenario of dynamically propagating cracks
provided a qualitative physical picture underlying the universality [1].

Industrial processes require also the fragmentation of polymeric materials which ex-
hibit ductile fracture. For polymers a complex deformation state may arise before breakup
which leads to a more complicated crack initiation and propagation compared to brittle
materials. In spite of its industrial relevance and scientific importance, the breakup of
polymeric materials is still poorly understood. In the present project we carried out a
detailed experimental and theoretical investigation of the impact fragmentation of poly-
mers which revealed a broad spectrum of novel features. Our experiments showed that
the mass distribution of plastic fragments exhibits a power law behavior with an expo-
nent close to 1.2, which is substantially different from the one of bulk brittle materials
in three-dimensions [9]. In order to understand the physical origin of the low exponent,
a three-dimensional discrete element model is developed where the sample is discretized
in terms of spherical particles connected by elastic beams. To capture the fracture mech-
anisms of plastic materials, in the model broken particle contacts are able to reconnect
when compressed against each other leading eventually to the healing of cracks. Computer
simulations revealed that the healing mechanism together with the dominance of shear
stresses in the crack formation are responsible for the emergence of the novel universality
class of fragmentation phenomena [9].

2 EXPERIMENTS

In the fragmentation experiments we used spherical particles made of polypropylene as
a test material. The most important physical properties of PP are summarized in Table
1. Mechanical properties of PP can easily be controlled by the temperature, providing ex-

| Table 1: Physical properties of polypropylene used in the experiments. |
|-------------------------|----------------|
| Young modulus     | 1300 MPa       |
| Glass transition temperature | -10 °C       |
| Melting point     | 160 °C         |
| Density           | 0.9 g/cm³      |

cellent possibilities to test the effect of mechanical properties on fragmentation processes.
For the purpose of the experiments a single particle comminution device was constructed
which accelerates particles one-by-one by the centrifugal force in a rotor up to the desired
velocity. The rotor ensures that the particles hit the hard wall at a rectangular angle
in an evacuated environment eliminating the disturbing effect of inclined impact and of
turbulent air flow. Experiments were carried out using Spherical PP particles of diameter
d = 5 mm which were impacted at different impact velocities v₀ in the range 30 m/s-180
m/s. Figure 1(a) demonstrates that at low enough velocities, the collision does not result in a breakup, instead the particles suffer a large plastic deformation at the impact site. Above the completely flattened contact zone meridional cracks form due to tensile stresses, however, the particle does not fragment. Most of the energy of the system is dissipated by plastic deformation of the particle. To obtain fragmentation the impact velocity \( v_0 \) has to exceed a material dependent critical value \( v_c \), which is about 60 m/s for our PP particles. For each impact velocity 400 particles were fragmented collecting the fragments in the grinding chamber of the machine. In the data analysis, 99 – 99.5% of the total mass of the samples was recovered. In order to evaluate the mass distribution of the fragments, we scanned the pieces with an open scanner obtaining digital images where fragments appear as white spots on the black background [7, 8] as it is illustrated in the inset of Fig. 2(a). Based on this technique the identification of fragments is reduced to searching of clusters of white pixels. We determined the two-dimensional projected area \( w \) of fragments as the number of pixels of the clusters, from which the mass \( m \) of fragments can be estimated as \( m \sim w^{3/2} \) since the three-dimensional fragment shape is close to isotropic. We carefully checked the shape isotropy by calculating the ratio of the two eigenvalues of the moment of inertia matrix of the projected area which always falls between 1 and 2.

Fig. 2 presents the mass distribution \( F(m) \) of fragments obtained at three different impact velocities. The inset shows an example of scanned fragments for the highest impact velocity. Note that due to the large number of fragments, the full experiment is composed of 4 such pictures comprising approximately 20000 pieces. It can be observed in Fig. 2 that at lower impact velocities a hump appears on the distribution function \( F(m) \) at the largest fragments which then gradually disappears as \( v_0 \) increases. The state of complete breakup is reached at the highest impact velocity \( v_0 = 75 \) m/s where the cutoff
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Figure 2: \((a)\) Mass distribution of fragments obtained from experiments at four different impact velocities. \(m_0\) denotes the average mass of PP spheres. At the highest impact velocity \(v_0 = 75\) m/s, \(F(m)\) shows a power law behavior over 3 orders of magnitude followed by an exponential cutoff for the very large pieces. Simulation results obtained with the parameters \(\Theta_{th} = 1\) and \(\iota_{th} = 0\) are in a very good agreement with the experimental findings. Inset: an example of scanned images of fragments for \(v_0 = 75\) m/s. \((b)\) The shape parameter of fragments determined from the scanned images. For most of the fragments the value of \(\sqrt{I_1/I_2}\) falls close to 1.9 which implies a high degree of isotropy of fragment shapes.

of the distribution becomes exponential and in the regime of small fragments a power law emerges

\[
F(m) \sim m^{-\tau_{pl}}
\]

over more than 3 orders of magnitude. It has to emphasized that the exponent \(\tau_{pl} = 1.2\pm0.06\) is significantly lower than the values \(\tau_{br} \approx 1.8-2.1\) obtained in the fragmentation of three-dimensional bulk objects made of disordered brittle materials [1, 2, 3, 4, 5]. The unique value of the exponent demonstrates that the breakup of plastic materials cannot be captured by the usual theoretical approaches.

3 DISCRETE ELEMENT MODEL

In order to obtain a detailed understanding of the physical mechanisms of the fragmentation of plastic materials, we used a Discrete Element Model (DEM) to simulate the fragmentation of a polymeric particles of spherical shape when they impact a hard wall. In the framework of the model the spherical sample is represented as a random packing of polydisperse spheres with a size distribution. Based on the initial particle positions a Delaunay triangulation is carried out in 3D which is used to determine the cohesive interaction of particles: the particles are connected by beam elements along the edges of the Delaunay triangulation such that not only those particles are connected which are initially in contact. The model construction is illustrated in Fig. 3(a) where the packing
of spheres and the connecting beam elements can nicely be observed. In the simulations the particles were composed of \( N \sim 24000 \) spheres.

In three-dimensional space the deformation of a beam is calculated by the superposition of elongation, torsion, as well as bending and shearing in two different planes [10]. In order to capture crucial aspects of the deformation behavior and the fracture of plastic materials, our DEM model has two novel types of components, i.e. the form of the breaking criterion of the beam elements and the reactivation of broken contacts under compression. Crack formation is implemented in the model such that the beams break when they get overstressed according to a physical breaking rule [9, 11]

\[
\frac{\varepsilon_1}{\varepsilon_{\theta \text{th}}} + \max (|\Theta_i|, |\Theta_j|) \geq 1.
\]  

(2)

In the breaking criterion \( \varepsilon \) denotes the longitudinal strain, furthermore, \( \Theta_i \) and \( \Theta_j \) are the generalized bending angles at the two beam ends [10]. Breaking of a beam can be induced by stretching and bending, the two terms of Eq. (2) characterize the contributions of the two failure modes.

Simulations showed that the local shear of the particle contacts provides the main contribution to the bending angles \( \theta_i, \theta_j \), so that bending dominated beam breaking in Eq. (2) characterizes crack formation due to shear. Varying the values of the breaking thresholds \( \varepsilon_{\theta \text{th}} \) and \( \theta_{\theta \text{th}} \), the relative importance of stretching and bending can be controlled: increasing the value of a breaking parameter, the effect of the corresponding failure mode diminishes. The extreme case of tension (stretching) dominance is achieved when \( \varepsilon/\varepsilon_{\theta \text{th}} \ll \theta/\theta_{\theta \text{th}} \), while the opposite case is the dominance of bending deformation in local failure events. An important feature of the breaking criterion is that in Eq. (2) the deformation \( \varepsilon \) is not restricted to positive values. Since the first term of Eq. (2) becomes negative when the beam is compressed, failure is dominated by the bending/shear mode in such a way that increasing compression increases the shear resistance of the beam. This scenario typically occurs for compressed contacts \( \varepsilon < 0 \) in the impact zone.

In order to represent the plastic behavior of the material in the framework of our DEM, we assume that the beams have a linearly elastic behavior up to fracture, but, whenever two particles are pressed against one-another for time longer than \( t_h \), a new, undeformed beam is inserted between them. This mechanism has the consequence that during the impact process, the particle contacts may undergo a sequence of breaking-healing events which leads to plastic energy dissipation and to the appearance of permanent deformation. Varying the healing time \( t_h \) the mechanical response of the model material can be controlled: \( t_h = 0 \) corresponds to the case of perfect shear plasticity, while \( t_h \to \infty \) implies no healing at all, i.e. brittle behavior.

4 COMPUTER SIMULATIONS

We carried out computer simulations of the impact process varying the impact velocity, the breaking parameters of beams, and the healing time over a broad range. Simulations
Figure 3: (a) In the framework of DEM the spherical sample is represented as a random packing of spheres which are connected by beam elements along the edges of a Delaunay triangulation in three dimensions. (b) At low enough impact velocities the samples suffers large permanent deformation but it does break. (c) Fragmentation is achieved when the impact velocity \( v_0 \) exceeds the critical velocity \( v_c \). In this regime the sample breaks into a large number of pieces. The simulation results are in a good quality agreement with the experimental findings.

were stopped when the system reached a relaxed state, i.e. when no beam breaking occurred during 1000 consecutive time steps. We control the effect of local failure modes of beams on the fragmentation process by setting the stretching threshold to a fixed value \( \varepsilon_{\text{th}} = 0.02 \) and we vary the bending threshold within a broad range \( 1.0 \leq \theta_{\text{th}} \leq 200 \). In this way \( \theta_{\text{th}} = 200 \) implies total tension dominance, while \( \theta_{\text{th}} = 1.0 \) means total bending dominance, and intermediate \( \theta_{\text{th}} \) values interpolate between the two limits.

In Fig. 3(b) and (c) final states of computer simulations are shown at a low and at a high impact velocity. At very low impact velocity the ball does not suffer any apparent damage, most of the impact energy is dissipated by the large permanent deformation at the impact site (Fig. 3(b)). In the limit of high impact velocity complete breakup occurs, the specimen falls apart into a large number of fragments (Fig. 3(c)). Figure 1 presents the comparison of the final state of a low-velocity impact simulation to the experimental finding. It can be observed that the model is able to reproduce both the deformation state and the crack structure of PP, with the parameter values where the beam breaking is dominated by bending \( \varepsilon_{\text{th}} = 0.02 \), \( \Theta_{\text{th}} = 1.0 \), furthermore, compressed contacts easily heal \( t_h = 0 \). It is interesting to note that the large permanent deformation of the ball in Fig. 1(b) is caused by the breaking-healing sequences of particle contacts. Above this zone tensile stresses arise resulting in opening cracks along the impact direction in agreement with the experiments [9].

Examples of the mass distribution of fragments are presented in Fig. 4 for two limiting parameter sets. In our model heterogeneous brittle materials are realized by the parameter values \( \Theta_{\text{th}} = 200 \), \( t_h = \infty \) for which a power law mass distribution is obtained with the usual exponent \( \tau_{br} = 1.9 \pm 0.1 \) [10]. Computer simulations showed that decreasing the healing time \( t_h \rightarrow 0 \) in the tension limit \( \Theta_{\text{th}} = 200 \) practically does not affect the fragmentation process because fragments are only generated by opening cracks which do
Figure 4: Mass distribution of fragments for two limiting cases of the parameter sets. In the regime of small fragment masses power law distributions are obtained, however, the value of the exponent depends on the dominating cracking mechanism. For tension dominated breakup the exponent $\tau_{br} = 1$ is obtained in agreement with the literature, however, for shear dominated breaking in the presence of plasticity a significantly lower exponent $\tau_{sh-pl} = 1.25$ emerges.

not let healing play a role. However, the breakup process substantially changes when shear dominates the crack formation $\Theta_{th} = 1$. At the same time increasing the strength of plasticity $t_h \rightarrow 0$ cracks formed at compressed contacts under shear can heal which then results in the merging of fragments. This mechanism has the consequence that the relative frequency of large pieces decreases leading to a faster decay of the distribution with a larger $\tau$. The exponent $\tau_{pl-sh} = 1.25 \pm 0.06$ presented in Fig. 4 is obtained in the plastic limit $t_h = 0$ together with $\Theta_{th} = 1.0$. The results of computer simulations are compared to the measured mass distribution of PP in Fig. 2. A very nice quantitative agreement can be seen which demonstrates that the shear dominated cracking together with the healing mechanism of compressed crack surfaces are responsible for the unique fragmentation of plastic materials. Our simulations indicate that the exponent $\tau_{pl-sh}$ is universal, i.e. it does not depend on details of the plastic mechanism or on the materials’ micro-structure characterizing a novel universality class of fragmentation phenomena [9].

Since particle contacts are sheared in the compressed zone in the vicinity of the impact site, a large fraction of the imparted energy is dissipated by the formation of small sized fragments and by the plastic deformation. Hence, the shock wave generated by the
impact leaves the destroyed zone with a low amplitude which hinders the expansion of the body and the appearance of meridional crack planes typical for the breakup of brittle spheres [10]. Due to the characteristic feature of low shear resistance, we find that the fragmentation of plastic shows similarities to the breakup of liquid droplets colliding with a hard wall. It can be observed in Fig. 3(c) that in the plastic-shear case the fragments escape laterally after impact indicating the “splash” of the entire body similar to liquid droplets [12, 13].

5 CONCLUSIONS

We carried out a detailed experimental and theoretical study of the fragmentation of plastic materials. In the experiments PP particles of spherical shape were impacted against a hard wall. In order to obtain a theoretical understanding of the emerging breakup process a Discrete Element Model was introduced which captured the main mechanisms relevant for fragmenting plastic. Our experimental and theoretical study revealed that the breakup of plastic materials falls into a novel universality class of fragmentation phenomena characterized by a unique value of the mass distribution exponent. Based on DEM simulations we showed that the plastic behavior of the material together with the dominance of shear in crack formation are responsible for the behavior substantially different from brittle fragmentation. It was found that the low shear resistance of the material results in a splashing mechanism similar to the breakup of liquid droplets.

Beyond the industrial importance of the fragmentation of polymeric materials, our results might be applied to obtain a deeper understanding of the fragmentation of highly viscous magma during pyroclastic activity at volcanic eruption [14, 15]. For theoretical investigations our results demonstrate that the breakup of solids cannot be understood as a generic stochastic process since the precise mechanism of crack initiation and growth, i.e. the dominance of tensile or shear stresses govern the process of fragmentation. Further investigations are in progress to determine the value of the critical exponents of the plastic fragmentation universality class.

REFERENCES


A FULLY COUPLED 3D TRANSPORT MODEL IN SPH FOR MULTI-SPECIES REACTION-DIFFUSION SYSTEMS

S. ADAMI\textsuperscript{a}, X.Y. HU\textsuperscript{a}, N.A. ADAMS\textsuperscript{a}, E.M. RYAN\textsuperscript{b} AND A.M. TARTAKOVSKY\textsuperscript{b}

\textsuperscript{a}Institute of Aerodynamics and Fluid Mechanics
Technische Universität München
85748 Garching, Germany
Corresponding author: stefan.adami@tum.de

\textsuperscript{b}Computational Mathematics Technical Group
Pacific Northwest National Laboratory
Richland, WA 99352, USA

Key words: SPH, Porous media, Reaction-diffusion

Abstract. In this paper we present a fully generalized transport model for multiple species in complex two and three-dimensional geometries. Based on previous work [1] we have extended our interfacial reaction-diffusion model to handle arbitrary numbers of species allowing for coupled reaction models. Each species is tracked independently and we consider different physics of a species with respect to the bulk phases in contact. We use our SPH model to simulate the reaction-diffusion problem on a pore-scale level of a solid oxide fuel cell (SOFC) with special emphasize on the effect of surface diffusion.

1 INTRODUCTION

In the context of global warming a lot of effort has been focused on developing renewable and alternative energy sources that reduce the production of greenhouse gases. A promising alternative energy technology, which converts chemical energy to electrical energy is the cold combustion in fuel cells. Amongst various realizations of this technology, solid oxide fuel cells (SOFC) are of special interest as their working conditions at high temperatures enable the usage of a wide variety of fuels [7]. Degradation is a central issue in SOFCs, such as chromium poisoning, which arises from the chromium contained in the stainless steel which is typically used for the current collectors. This chromium reacts with air to form volatile chromium species that [8] migrate into the porous cathode and react with its surface. This so-called chromium poisoning has been shown to decrease the efficiency of the fuel cell dramatically and has to be controlled [6].
Ryan et al. [12] have developed a pore-scaled SPH model of a SOFC to investigate the reactive transport of chromium species in the cathode. Based on a multi-scale approach including a cell level model of the cathode, air channel and the current collector they determined the boundary conditions for the pore scale simulations. In their two-dimensional work they varied the reaction rates of oxygen and chromium and the working conditions of the fuel cell to study the deposition of chromium. They could reproduce qualitatively the species distributions in the cathode as compared to experimental findings [6] and show that their nonlinear competitive adsorption-desorption model is adequate to study the complex chromium poisoning.

In our current work we want to use the competitive adsorption-desorption model to simulate the chromium deposition in a realistic three-dimensional cathode. Different from the two-dimensional study of Ryan et al., here we cannot neglect surface diffusion in the porous material as this structure allows an interfacial connection throughout the entire domain and diffusion along the interface can alter the species dynamics strongly.

To simulate a multi-component reactive transport problem we have extended our SPH method for surfactant dynamics [1] to account for multiple species and coupled transport models. We have validated this method with analytical solutions for coupled transport-diffusion systems with different boundary conditions (Neumann, Dirichlet and Robin) and demonstrate the significance of surface diffusion for the species transport in a real porous cathode structure.

2 GOVERNING EQUATIONS

Briefly we recall the governing equations of the fluid and species dynamics in a porous structure in a very general form. From mass conservation we can formulate the continuity equation in the form

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \bar{u},$$

where $\rho$, $\bar{u}$ and $t$ denote the density, the velocity vector and the time, respectively. The momentum equation in Lagrangian form with the pressure $p$, a bodyforce $\bar{g}$ and the dynamic viscosity $\eta$ is given by

$$\rho \frac{d\bar{u}}{dt} = -\nabla p + \rho \bar{g} + \nabla \eta \nabla \cdot \bar{u}.$$  

An advection-diffusion equation is used to describe the dynamics of a species $\alpha$ in a bulk phase $l$ according to

$$\frac{dm^\alpha_C}{dt} = \int \nabla D^\alpha_\infty \nabla C^\alpha \; dV - \int S^\alpha_\Sigma \delta^\Sigma \; dV.$$  

Here, $m^\alpha_C$ and $C^\alpha$ denote the mass and mass concentration of the species $\alpha$ in the bulk. Assuming isotropic bulk diffusion the diffusion tensor $D^\alpha_\infty$ reduces to the scalar diffusion coefficient $D^\alpha_\infty$. Note that the bulk diffusion can vary for each species in different bulk
phases, i.e. the diffusion coefficient $D_\infty^\alpha$ is a function of the species type $\alpha$ and the bulk phase where it is dissolved. The last term in (3) represents the transport of species $\alpha$ from/to the bulk phase to/from an interface it is in contact with. In continuous form the source term $S_\Sigma^\alpha$ on the interface $\Sigma$ is integrated in the domain via the surface delta function $\delta_\Sigma$.

On the interface we account for surface diffusion and species transport via

$$\frac{d m_\Gamma^\alpha}{dt} = \int \nabla_s D_s^\alpha \nabla_s \Gamma^\alpha \delta_\Sigma \, dV + \int \dot{S}_\Sigma^\alpha \delta_\Sigma \, dV,$$

where $m_\Gamma^\alpha$, $\Gamma^\alpha$ and $D_s^\alpha$ are the mass and mass concentration of species $\alpha$ on the interface $\Sigma$ and the surface diffusion coefficient (again assuming isotropic surface diffusion). Note, the surface gradient operator $\nabla_s$ can be written as $(I - \mathbf{n} \otimes \mathbf{n}) \nabla$, which will be used later. The second term in (4) is equivalent to the source mass flux in the species balance equation in the bulk phase (3) to ensure mass conservation of each species.

The surface transport model in a very general form is given by

$$\dot{S}_\Sigma^\alpha = f \left( C^1, C^2, ..., C^\alpha, \Gamma^1, \Gamma^2, ..., \Gamma^\alpha \right).$$

Here, the source term $\dot{S}_\Sigma$ is a function of the surface concentrations $\Gamma$ and the bulk concentrations $C$ adjacent to the interface of all species $\alpha$ in the system. We implemented this general formulation to include arbitrarily complex transport models starting from the most simple no flux condition $\dot{S}_\Sigma^\alpha = 0$ up to coupled competitive reaction models such as the Langmuir model [14].

3 NUMERICAL METHOD

Generally, the equations of motion for a Lagrangian fluid element can be integrated in time with the SPH method as presented in [10]. In the weakly-compressible approach the unknown pressure in the fluid phase is calculated from the density via an equation of state in the form

$$p = p_0 \left( \frac{\rho}{\rho_0} \right)^\gamma,$$

where the reference pressure $p_0$ and density $\rho_0$ together with the exponent $\gamma$ are chosen according to a scale analysis to limit the maximum density variation, see [11]. As we do not evolve the flow quantities of the fluid in this work we do not further explain the details of our flow solver but concentrate on the species model. The simplification of neglecting advection to study the competitive reaction-diffusion problem in a porous structure is justified by the work of [12], who showed that advection processes in the cathode are insignificant for the chromium poisoning.

We discretize the domain of interest with Cartesian particles with an equidistant spacing of $\Delta x$. Consequently, the volume of a particle $i$ is $V_i = \Delta x^n$ with $n$ denoting the number of dimensions. The quintic spline kernel [11] is used as smoothing function $W$.
with a cutoff radius \( r_c = 3h \), where the smoothing length \( h \) is set to the initial particle distance. Following the multi-phase model of [9], we introduce a color function \( c \) that defines if a particle \( i \) belongs to a phase \( l \) \((c_i^l = 1)\) or not \((c_i^l = 0)\). Using this color function phase interfaces are defined implicitly as the color gradient \( \nabla c \) is non-vanishing only in a transition band of thickness \( r_c \) along the interface. Within this transition band, the governing equations for the surface dynamics of the species are solved locally for each individual particle.

As the interface singularity is represented by a continuous surface delta-function (here the magnitude of the color-gradient function \(|\nabla c|\) is used as \( \delta_\Sigma \)) every particle in the narrow band along an interface contributes to the interface area by

\[
A_i = |\nabla c_i| V_i . \tag{7}
\]

Correspondingly, every interface particle carries a fraction of the mass of species \( \alpha \) accumulated on the interface \( m^\alpha_i = \Gamma^\alpha_i A_i \). As the interface singularity is discretized by a transition band of finite thickness, we can use the derivations of [3] and solve the surface diffusion equation in continuous form for every interface particle as

\[
\frac{d\Gamma^\alpha_i}{dt} = \frac{1}{|\nabla c_i|} \nabla \cdot \left([\mathbf{I} - \mathbf{n}_i \otimes \mathbf{n}_i] D_s^\alpha \nabla \Gamma^\alpha_i |\nabla c_i| \right) . \tag{8}
\]

The normal direction at the interface \( \mathbf{n}_i \) is found from an averaging of the normalized color-gradient vectors of neighboring interface particles. Finally, the rate of change of the interfacial mass \( m^\alpha_i \) due to surface diffusion is obtained by

\[
\frac{dm^\alpha_i}{dt} = \sum_j \left( \lambda^\alpha_i V_i^2 + \lambda^\alpha_j V_j^2 \right) \nabla W (\mathbf{x}_i - \mathbf{x}_j) . \tag{9}
\]

The summation is over all neighboring particles \( j \) that contribute to the interface and \( \lambda^\alpha \) is the flux of species \( \alpha \) projected in tangential surface direction at particle \( i \) \((\lambda = (\mathbf{I} - \mathbf{n}_i \otimes \mathbf{n}_i) D_s^\alpha \nabla \Gamma^\alpha_i |\nabla c_i|)\). At the fringes of the transition band the surface gradient of a species concentration cannot be calculated with a general SPH gradient formula as the contributing interface particles do not provide full support for the summation. As a remedy, we can approximate the gradient on the interface by a summation only with interface particles as given by

\[
\nabla \Gamma^\alpha_i = \frac{\sum_j (\Gamma^\alpha_i - \Gamma^\alpha_j) \nabla W_{ij}}{\sum_j r_{ij} \frac{\partial W}{\partial r_{ij}}} \tag{10}
\]

with \( r_{ij} = |\mathbf{x}_i - \mathbf{x}_j| \). For details of the derivation and accuracy of this form we refer to [2].

The evolution of the surface mass of a species due to exchange with the bulk phase for each interface particle is simply \( \frac{dm^\alpha_i}{dt} = \dot{S}_\Sigma^\alpha |\nabla c_i| V_i \). The surface concentration is
updated in time by
\[ \Gamma_i^\alpha = \frac{\sum_j m_{ij}^\alpha W_{ij}}{\sum_j A_j W_{ij}}, \]  
(11)
where the summation is performed over all neighboring interface particles. This additional averaging step is required as a simple local estimation could cause numerical instabilities due to very small interfacial contributions of particles close to the fringes of the interfacial transition band.

The presented model is based on a so-called two-sided physics assumption, i.e. the transport and diffusion phenomena are solved numerically on a layer adjacent to the interface of both phases. There are situations where one phase cannot dissolve a species but the surface transport model includes desorption of surface material to the other bulk phase. Then, we apply some special mapping techniques to ensure exact conservation of the species and to consider the total interfacial area. Further information of this special computational aspect can be found in [1]. A similar model for the one-sided problem has been proposed and validated in [13] for reactive transport problems with surface reactions.

The SPH approximation of the bulk diffusion equation in conservative form can be expressed as
\[ \frac{dm_i^\alpha}{dt} = \sum_j \frac{2D_{\infty i}^\alpha D_{\infty j}^\alpha}{D_{\infty i}^\alpha + D_{\infty j}^\alpha} \left( V_i^2 + V_j^2 \right) \frac{C_i^\alpha - C_j^\alpha}{r_{ij}} \frac{\partial W}{\partial r_{ij}}. \]  
(12)
Note that the inter-particle averaged diffusion coefficient in (12) satisfies the no-flux condition between two particles if the species is insoluble in one of the phases. Additionally, the bulk species mass of a particle close to an interface changes due to the adsorption and desorption at the interface as \( \frac{dm_i^\alpha}{dt} = -\dot{S}_{\Sigma i}^\alpha |\nabla c_i| V_i. \)

The anti-symmetry of the discretized transport equations in the bulk phase (12) and on the interface (9) on the local particle-interaction level ensures exact global species mass conservation.

We have presented a method to simulate multi-species reaction-diffusion problems on complex geometries with SPH. Generally, the equations hold for arbitrary numbers of species \( \alpha \) each following different physical models. But with increasing variety the computational effort increases as for every species the transport model coefficients such as surface diffusivity or adsorption constants have to be defined separately for every interface combination and bulk phase. So far, we have not yet specified a transport model for the source term \( \dot{S}_{\Sigma i}^\alpha \) in the species evolution equation as any functional form including the local bulk and surface concentrations can be used. We present the employed transport models in the next section where we show some validation cases. Finally, we study the coupled species dynamics on a realistic three-dimensional porous structure of a SOFC cathode.
We solve the diffusion problem in a hollow cylinder with different boundary flux conditions to validate our model. A sketch of the problem is given in Fig. 1. At the outer radius \( R_o \) the species concentration is set to \( C_0 \) for all times and at the inner radius \( R_i \) different boundary flux conditions are tested. Initially, the concentration in the hollow cylinder is \( C(t = 0) = 0 \). The inner and outer radii are \( R_i = 1 \) and \( R_o = 2 \) and we discretize the geometry with Cartesian SPH particles with \( \Delta x = 0.05 \), i.e. we use 20 particles in radial direction. We compare our results with the analytical solution for bulk diffusion in a hollow cylinder with a flux boundary condition given by [5].

\[
\nabla \cdot \mathbf{C} = q(13)
\]

4.1 Neumann boundary condition

At first we apply a Neumann boundary condition at the inner radius

\[
D \nabla C \big|_{R_i} \cdot \mathbf{n} = q_0
\]

with the constant flux \( q_0 \). When we rewrite the boundary condition in terms of a transport model to/from the interface, the source term in the species evolution equation is \( S_C = q_0 \).

Fig. 2 shows spatial concentration profiles over time in the bulk phase with \( D = 1 \). In this special case we set \( q_0 = 0 \), i.e. a no-flux boundary condition at the inner radius. The agreement with the analytic result is good and the accuracy increases with resolution.

Now we use a constant boundary flux \( q_0 = 0.1 \) to validate the mass transport at an interface. Again, good agreement and convergence is found when comparing the simulations with the reference solution, see Fig. 3. Not shown here, we also monitored the mass accumulated at the interface due to the boundary flux and found exact global conservation for our transport model.

4.2 Robin boundary condition

Now we test a more complex linear Robin boundary condition of the form

\[
D_\infty \nabla C \cdot \mathbf{n} = K (C - C_{eq})
\]
Figure 2: Radial concentrations over time in the hollow cylinder for the no-flux boundary condition at $R_i$.

Figure 3: Radial concentrations over time in the hollow cylinder with a Neumann boundary condition at $R_i$.

with the equilibrium concentration $C_{eq}$ and a reaction rate $K$. In this case we use $D = 0.1$, $C_{eq} = 0.5$ and $K = 1$. The radial concentration profiles over time are shown in Fig. 4.

Figure 4: Radial concentrations over time in the hollow cylinder with a linear Robin boundary condition at $R_i$.

Figure 5: Temporal surface concentration profile for two species $oxy$ and $chr$ for a competitive adsorption model.

As the initial bulk concentration is zero, according to the boundary condition (14) a negative flux injects mass to the bulk phase at the inner radius. Consequently, the concentration profile is different from the previous diffusive profiles as species material is transported to the inner regions by the boundary flux and not only via diffusion from the outer radius. At very late times, the concentration at the inner interface approaches the equilibrium value of the Robin condition $C_{eq}$. 
4.3 Competitive adsorption-desorption model

So far we have simulated uncoupled problems, i.e. each species is independent of the other ones. Now we use the modified Langmuir model [14] to simulate competitive adsorption of two components. The non-linear source terms for the two species oxy and chr are

\[
\dot{S}_\Sigma^{oxy} = k_1^{oxy} C_\infty^{oxy} \left[ 1 - \Gamma^{oxy} - \Gamma^{chr} \right]^2 - k_2^{oxy} (\Gamma^{oxy})^2 \\
\dot{S}_\Sigma^{chr} = k_1^{chr} C_\infty^{chr} \left[ 1 - \Gamma^{oxy} - \Gamma^{chr} \right]^3 - k_2^{chr} (\Gamma^{chr})^3.
\]

(15) (16)

We simulate the adsorption process from a bulk phase to a circular interface with radius \( R = 1 \). We assume diffusion to be much larger than the surface reaction rates, i.e. the bulk concentrations \( C_\infty^{oxy} = 1 \) and \( C_\infty^{chr} = 1 \) are both constant in time. For simplicity we set all reaction constants \( k_1 \) and \( k_2 \) to unity and use the same discretization as in the previous examples.

From our parameter setup we find an equilibrium for both species concentrations at

\[ \Gamma^{oxy} = \Gamma^{chr} = \frac{1}{3} \]

(17)

where the surface reaction is balanced and a steady-state is reached. In Fig. 5 we show the temporal evolution of the averaged surface concentrations for both species. We compare our results with a quasi-onedimensional high resolution finite-difference calculation using a fourth order Runge-Kutta integration scheme and very good agreement is found. In the beginning, adsorption of species oxy is faster than species chr and an overshoot of the equilibrium condition occurs. Later, both components reach the steady equilibrium state and the net surface flux is zero.

5 POROUS Structure

We have demonstrated the validity of our method to simulate complex surface transport problems on curved interfaces in two dimensions. Now we want to study a more realistic three-dimensional reaction-diffusion problem in a porous structure as it occurs in a SOFC cathode. For that purpose we take a pixelmap of a section of a real cathode structure provided by the Pacific Northwest National Laboratory and discretize the pores and the air phase with different types of particles, see the red (pores) and blue (air) particles in Fig. 6.

Using the color-function gradient between the two phases to determine the interface position, we can reconstruct the surface of the pores and simulate the interfacial diffusion of a scalar species coupled with bulk transport. Fig. 7 shows the reconstruction of the interface using our SPH discretization of the problem. The non-dimensional size of the geometry is \( 32 \times 32 \times 16 \) and we have used a particle spacing of \( \Delta x = 0.25 \). Thus a total of 1,048,576 particles is used.
As we are interested in the impact of surface diffusion, we do not simulate an entire fuel cell with an air channel, current collector, anode and cathode but study the species dynamics in a section of the cathode to estimate time scales and the influence of reaction rates and surface diffusion on the distribution of a species in the cathode. Then we can use these results to improve continuous coarse-grid models for porous media and study the depositioning of chromium in a real cathode.

In this work we compare three simulations with an isolated species at different diffusion rates to demonstrate that surface diffusion can strongly change the dynamics of the poisoning. The Langmuir adsorption-desorption model given by

\[ \dot{S}_\Sigma = k_1 C (\Gamma_{\text{max}} - \Gamma) - k_2 \Gamma \]  

is used for the surface transport with the parameter \( k_1 = 1.0 \), \( k_2 = 0.2 \) and \( \Gamma_{\text{max}} = 1.0 \). At the top layer we define the bulk concentration of chromium \( C_\infty = 1.0 \), constant in time. We impose symmetry boundary conditions in x and y direction as periodicity cannot be applied to a heterogeneous porous structure. Also the flux of species along the sidewise boundaries was shown to be marginal, hence negligible \([12]\) which verifies the symmetry assumption. The bottom of the cathode section is impermeable for chromium and we use a no-flux boundary condition there.

Table 1 shows the parameters for the surface and bulk diffusion of our simulations. Case 1 is dominated by a strong bulk diffusion, in Case 2 we amplified the surface diffusion and Case 3 is used as a reference result to estimate the effect of the two variations.

In Fig. 8 - 10 snapshots of the three simulations at \( T = 8 \) show a section of the interface and a slice through the bulk phase to show the surface concentration and the bulk concentration. The colors in the figures show the quantities from blue to red in the range of \( \Gamma = 0 - 0.833 \) and \( C = 0 - 1 \), respectively.
Table 1: Diffusion coefficients for the three cases.

<table>
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<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_s$</td>
<td>0.1</td>
<td>1.0</td>
<td>0.1</td>
</tr>
<tr>
<td>$D_\infty$</td>
<td>10.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

From these figures we see immediately the influence of bulk diffusion on the species distribution in the gas phase. The penetration depth of chromium in the bulk (Fig. 8) is larger than for the other cases. Interestingly, the surface concentration distribution is similar for Case 1 and Case 2 although the diffusion rates are inverse. To further analyse the results we postprocessed the concentration profiles and calculated average interface and bulk concentrations in small slices along the z-axis. Of course diffusion in the porous media is not uniform and not quasi-onedimensional in the z-direction, but from the averaged profiles we can better interpretate the results and describe qualitatively the effect of different parameter.

The averaged bulk concentration profiles in the z-direction at $T = 8$ for the three different cases are shown in Fig. 11. At the upper boundary at $z = 16$ the concentration is equal to the reference value and for the high bulk diffusivity the biggest amount of chromium mass is deposited into the porous structure. Correspondingly we show the averaged surface concentration in slices along the z-axis for all cases in Fig. 12. As a reference, we have also plotted the equilibrium surface concentration for the reference bulk concentration obtained from

$$
\Gamma_{eq} = \frac{k_1 \Gamma_{max} C_\infty}{k_1 C_\infty + k_2}.
$$

Close to the upper boundary, the surface concentration has already reached the equilibrium value and remains constant in time. The dots in this figure show the profile of the equilibrium surface concentration calculated from (19) using the local averaged bulk con-
centrations. Comparing the actual local profile and the theoretical equilibrium profile for Case 1 we see that diffusion rates are much faster compared to the transport to the surface. Thus, the surface concentration in lower regions did not yet achieve the equilibrium condition as the adsorption rate is too small.

Moreover we want to emphasize that the two bulk concentrations of Case 2 and Case 3 differ considerably although the bulk diffusion coefficient is equal for both setups. This effect can be explained together with the surface concentration profiles and the Langmuir model. Looking at Case 3, the surface concentration profile coincides with the calculated equilibrium profile. That means chromium diffuses slowly through the bulk phase and almost instantaneously the surface reaction is in equilibrium with the bulk phase.

The bulk diffusion in Case 2 is equivalent with Case 3, but much more material is already transported to the air phase in the cathode and the averaged bulk concentration profile in Fig. 11 is higher. This material comes from the desorption of chromium from the interface. The high surface diffusivity transports chromium along the interface into the structure. Consequently, the surface concentration gradient is smoothed stronger and even at the upper boundary the interface equilibrium condition is not yet reached. In addition, desorption takes place lower in the structure since the interface is oversaturated according to (19) and chromium occurs in a depth where pure bulk diffusion could not yet transport material.

6 CONCLUSION

We have presented a fully coupled multi-species SPH model considering the effect of surface diffusion, surface reaction and bulk diffusion. The validation against analytical and high-resolution results shows very good agreement and convergence of our method is proved. We used our method to simulate the complex interaction of surface diffusion, reaction and bulk diffusion in a three-dimensional porous structure of a real cathode of
a fuel cell and highlight the deposition of chromium into the cathode via surface diffusion. In future work we want to explore a more complex coupled two-species transport model to represent the competitive species dynamics of oxygen and chromium and use more realistic boundary conditions such as prescribed flux conditions and concentration dependent reaction rates.

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REFERENCES


PARTICLE HYDRODYNAMICS: FROM MOLECULAR TO COLLOIDAL FLUIDS

F. Balboa-Usabiaga, R. Delgado-Buscalioni
Departamento de Física Teorica de la Materia Condensada.
Universidad Autónoma de Madrid
Campus de Cantoblanco, Madrid 28049
e-mail: rafael.delgado@uam.es

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Abstract. A method for particle hydrodynamics based on an hybrid Eulerian-Lagrangian approach is presented. Particles are solved in the continuum space while the fluid is solved in an Eulerian mesh, and described by finite volume fluctuating hydrodynamics. This set-up is particulary suited for micron-size devices where the Reynolds number is small but thermal fluctuations are important. The fluid-particle coupling force is obtained by imposing zero relative (particle-fluid) velocity at discrete points representing the particle sites. In this work particles are described by an only site which neglect rotation. The momentum exchanged between fluid and particle is transfered instantaneously and this brings about several benefits such as a correct treatment of inertia and proper particle velocity fluctuations uniquely driven by the fluid thermal forces. The present scheme is designed for incompressible and compressible fluids at low Mach number. This is theoretically shown by analyzing the consistency between the Eulerian and Lagrangian momentum balance. A series of tests up to moderate Reynolds number and acoustic forces under ultrasound waves are also presented.

1 INTRODUCTION
The emergence of complex phenomena is common aspect in particle hydrodynamics. An example is the collective motion of a swarm of particles immersed in a fluid, interacting among them with short-ranged potentials and also along larger distances, via the hydrodynamic field [1]. Numerical simulations constitute a powerful tool to isolate and dissect the effect of each force or detail, in ways that cannot be experimentally reproduced. Computational studies of this sort certainly requires some type of simplification or coarse-graining procedure. A hierarchical list of simplifications might be envisaged, starting from the elimination of the molecular degrees of freedom of the solvent and concluding by the
gradual simplification of the solute particle structure up to a single “point” moving in space (the so called point particle approximation [2]). In performing this reductionist approach one needs to consider several important constraints: consistent momentum (and energy) conservation and hydrodynamic fluctuations if dealing with micron or submicron size systems (in such case convection does not make a significant contribution).

There are three general schemes to face the general problem of particle hydrodynamics: fully Eulerian, fully Lagrangian methods and Eulerian-Lagrangian hybrids. Treating both particle and solvent within an Eulerian grid demands solving the delicate technical problem of adapting the grid (remeshing) around the moving particle. A more natural approach might be to use fully Lagrangian schemes, based for instance in Smooth Particle Hydrodynamics. These have been evolving in complexity and have been recently generalized to non-Newtonian fluids [5]. Here we focus on the third approach whereby the fluid is solved in the (probably faster) fixed Eulerian grid, while particles move in the continuum space. Ideas from these three approaches start to spread (SPH with remeshing steps are now used [6] and maybe, SPH interpolation kernels could adapted to Eulerian-Lagrangian methods).

The kernel function is key to properly solve the particle hydrodynamics. It is in charge of the two essential communications: how to spread local (surface or point) forces over the fluid and how to interpolate fluid variables at desired (particle) point. We adhere to the interpolation kernels derived for the Immersed Boundary method [7] and show they are flexible enough to ensure consistency in the force and velocity coupling. Another key issue is the ansatz used for the particle-fluid force. This determines the physics the method will be able to tackle. In particular, in the IB method the particle (or surface point) velocity \( \dot{\mathbf{R}} \) simply follows the local fluid interpolated value \( \mathbf{u} \), meaning that inertial forces are absent. The exchanged forces arise from the distortion of the particle-particle potential energy as in fact, an isolated particle would have trivial \( \dot{\mathbf{R}} = \mathbf{u} \) dynamics. If one is interested in tracing non-bonded particles another strategy is thus required. A common one is to construct a force inspired on the zero Reynolds form of the Stokes drag, \( \mathbf{F} = \xi(\dot{\mathbf{R}} - \mathbf{u}) \), providing a fluid-particle force and non-trivial dynamics \( \dot{\mathbf{R}} = \mathbf{F}/M \) for particle with mass \( M \). If fluctuations are important, the damping force used for the particle-fluid coupling makes necessary the usage of a noise term in the particle equation to ensure the correct equilibrium kinetic temperature of the particles [2]. The Stokes coupling introduces a friction time \( M/\xi \) which limits the fastest process one can resolve. A number of interesting applications of polymeric and colloidal suspensions in micro-flow devices however require relative large flow change rates and velocity gradients of the same order of the particle radius for which the Stokes friction limit neither valid. Applications involving ultrasound are now flourishing, such as manipulation or treatment of micron size particles using ultrasound, with important technological applications [3]. In this report we present an extension to the above ideas where particle and fluid motion are coupled in the strongly overdamped limit, i.e. the fluid-particle transfer of momentum is instantaneous. This method, called Direct Forcing, obtains the fluid-particle force upon imposition of
the no-slip fluid velocity at a single particle site. This work extends previous Direct Forcing approaches [4] to point-wise particles, giving a precise meaning of the particle effective volume, and comparing for consistency the Eulerian and Lagrangian versions of momentum conservation.

2 Equations of motion

Consider an spherical particle of mass $M_p$ immersed in a fluid. The particle center is located at $\mathbf{R}_p(t)$, it has surface $S_p$ and volume $V_p$. The force on the particle due to the fluid is given by the sum of the fluid pressure over the particle surface, $-\oint_{S_p} \mathbf{P} \cdot \mathbf{n} dr^2$.

Using the divergence theorem, the particle equation of motion results in

$$M_p \frac{d\mathbf{V}_p}{dt} = -\int_{V_p} \nabla \cdot \mathbf{P} dr^3 + \mathbf{F}_{\text{ext}}$$

(1)

where $\mathbf{V}_p = \dot{\mathbf{R}}_p$. An extra force $\mathbf{F}_{\text{ext}}$ has been added to represent any external field and/or interaction with other particles. In what follows we focus on particle translation and ignore particle rotation. Extensions to include rotational degrees of freedom are underway. We also consider a Newtonian fluid in isothermal environment for which the conservation equations of mass density $\rho(r, t)$ and momentum density $\mathbf{g}(r, t) = \rho \mathbf{u}$ are

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{g}$$

(2)

$$\frac{\partial \mathbf{g}}{\partial t} = -\nabla \cdot \mathbf{\Pi} + \mathbf{f}.$$  

(3)

Where the stress tensor $\mathbf{\Pi} = \mathbf{g} \mathbf{u} + \mathbf{P}$ includes the convective term and $\mathbf{P} = \pi \mathbf{1} + \eta [\nabla \mathbf{u}]^{\text{sym}} + \bar{\mathbf{P}}$ contains an scalar pressure $\pi$ a diffusive term (the symmetrized tensor is indicated as $A^{\text{sym}} = (A + A^T)/2$) and a fluctuating component of thermal origin. Fluctuating hydrodynamics described by Eqs. (2) and (3) were solved using the finite volume method in a regular mesh. Details can be found in Ref. [8]. In general, the density force $\mathbf{f}$ arises from the fluid-particle interaction, ensures fulfillment of the velocity boundary condition at the particle surface and the exclusion of fluid from the particle inside. These boundary equations require resolving the particle surface (using a set of points at the surface) [4]. By contrast the intention here is to simplify the particle description up to being described by a single point at its center and an effective volume $V_p$. The boundary condition for the fluid velocity is thus,

$$\mathbf{u}(\mathbf{R}_p) = \mathbf{V}_p$$

(4)

where $\mathbf{V}_p = \dot{\mathbf{R}}_p$ is the particle velocity. Finally in this point-wise approximation, the fluid leaks into or entrain the particle. In other words, no boundary condition is imposed inside or at the particle domain.
2.1 Force balance and momentum conservation

Instead of directly dealing with the integral of the divergence of the pressure tensor to solve the particle dynamics described by Eq. (1), it is much easier to reformulate the problem in terms of global momentum conservation. More generally, consider that the fluid contains a number of particles \( p = \{1, \ldots, M\} \) located at \( \{R_p\} \). One can integrate Eq. (3) over the whole domain to obtain the rate of change of total fluid momentum

\[
\frac{d}{dt} \int g \, dr^3 = \int \nabla \cdot \mathbf{P} \, dr^3 + \int f \, dr^3
\]

(5)

We shall assume that the fluid-particle interaction is local and short ranged, with a cutoff radius of microscopic size. This means that the force \( f \) only differs from zero around a shell infinitely close to each particle surface. The volume of this shell around one particle \( p \) is denoted \( V_p \). Under this assumption

\[
\int f \, dr^3 = \int_{V_p} f \, dr^3 = \sum_p \int_{V_p} f \, dr^3.
\]

(6)

For the last equality we assume non-overlapping particle volumes, which follows from the fact that particles cannot interpenetrate. The total force due to particle \( p \) is denoted as, \( F_p = \int_{V_p} f \, dr^3 \) so that the total force on the fluid due to the particles is

\[
\sum_p F_p = \int f \, dr^3
\]

(7)

To derive a dynamic equation for the particle \( p \) we integrate Eq. (3) over the particle volume \( V_p \) and insert Eq. (1) to get,

\[
M_p \frac{dV_p}{dt} = \frac{d}{dt} \int_{V_p} g \, dr^3 - \int_{V_p} f \, dr^3 + F_{\text{ext}}
\]

(8)

For an incompressible fluid of density \( \rho \), momentum conservation inside the particle ensures that \( \frac{d}{dt} \int_V g \, dr^3 = \rho \frac{d}{dt} [\int_V \mathbf{u} \, dr^3] = m_p \frac{dV_p}{dt} \) where the \( m_p = \rho V \) is the fluid mass the particle evacuates. The Archimedes force is thus recovered,

\[
\Delta M_p \frac{dV_p}{dt} = -F_p + F_{\text{ext}}
\]

(9)

The mass excess \( \Delta M_p = M_p - m_p \) is indeed constant for an incompressible fluid, so fixing \( \Delta M_p \) means defining the particle mass \( M_p = \Delta M_p + \rho V \). In Eq. (9) we have defined \( F_p \) as the total force exchanged between the fluid and the particle \( p \). Note that Eq. (9) ensures that the total momentum of the system is conserved.
2.2 The particle-fluid force

As stated, the central idea of the direct forcing scheme is to obtain the fluid-particle interaction force $F_p$ from the imposition of the no-slip boundary condition at the particle site $R_p$. As particles do not overlap, the total force exchanged between the fluid and the whole set of particles is just the sum of each individual particle contribution, as stated in Eq. (7). Let us then derive the force due to one particle $p$. The fluid momentum variation due to such force $F_p$ over time interval $\Delta t$ is given by the integral of Eq. (3) over $V_p$ and $\Delta t$. Let us now focus on incompressible fluids $g(r) = \rho u(r)$ to get,

$$
\rho (u)_p(t + \Delta t) = \rho \tilde{u}_p + \frac{1}{V_p} \int_{t}^{t+\Delta t} F_p(t') dt'.
$$

Equation (10) also introduces,

$$
\rho \tilde{u}_p = \rho (u)_p(t) - \int_{t}^{t+\Delta t} (\nabla \cdot \Pi)_p(t') dt',
$$

which is the average momentum density that fluid would have had in the particle domain if no particle constraint would have been imposed during the time interval. In this sense $\tilde{u}$ is called unperturbed fluid velocity. Imposing the “stick” constraint $(u)_p = V_p$ in Eq. (10) yields the following integral restriction to the force,

$$
\int_{t}^{t+\Delta t} F_p(t') dt' = \rho V_p [V_p(t + \Delta t) - \tilde{u}_p].
$$

Equation (12) is the change of fluid momentum over $\Delta t$ due to the presence of the particle $p$. Generalization to many non-overlapping particles is straightforward, as stated in Eq. (7).

3 Implementation

Equations (5)-(12) constitute the core of the particle hydrodynamics problem we intend to solve. To that end, the next ingredient to add is the so called “point-particle” approximation, which formally consists on approximating the volume average $\langle \phi \rangle_p$ by an interpolated value $\phi_p$ at some location (for spherical particles in incompressible fluid, the particle center) in the particle domain $V_p$. For this task we use the kernel function developed for the Immersed Boundary Method (IBM)[7]. On the other hand, in this work we use a first order explicit scheme (forward Euler) to integrate the equations in time. Both issues are now discussed.
3.1 Interpolation and Spreading

The Eulerian-Lagrangian mixed approach moves the particle in the continuum (Lagrangian) space while the fluid is solved in a fixed Eulerian mesh. Any Eulerian fluid solver (based either on finite differences, finite volumes or even the Lattice-Boltzmann method) can be used. The set of \( i = \{1, ..., N\} \) fluid nodes are located at \( \{r_i\} \) fluid nodes. On the other hand there are \( p = \{1, ..., M\} \) particles at sites \( \{R_p\} \). Communication between Eulerian and Lagrangian dynamics require two central operations. First, the evaluation of the fluid-particle force in Eq. (12) requires the interpolation of the unperturbed fluid velocity at the particle site and, second, this force has to be spread to the surrounding fluid nodes (so that Eq. (10) is fulfilled at each particle site). These two operations are respectively performed by the operators \( \delta^I(s) \) and \( \delta^S(s) \) which can be generally defined as convolution integrals in the continuum space [7]. As we are focusing on discrete (point-wise) particles it is more natural to express these operations in its discrete form,

\[
\phi^I_p = \sum_i \delta^I_{ip} \phi_i \quad \text{and} \quad \phi^S_i = \sum_p \delta^S_{ip} \phi_p
\]

where \( \phi_i = \phi(r_i) \) and \( \phi_p = \phi(R_p) \). The spreading and interpolators are constructed like \( \delta^I(r) = \delta_h(x) \delta_h(y) \delta_h(z) \) where \( \delta_h(s) \) is the three point kernel discussed in Ref. [7]. In any case \( \delta^I_{ip} = \delta^I(|r_i - R_p|) \) (similarly for \( \delta^S \)). The following properties hold:

\[
\sum_i h^3 \delta^I_{ip} = h^3 \quad \text{(14)}
\]

\[
\sum_i h^3 \delta^S_{ip} = V_p \quad \text{(15)}
\]

It is also particularly important that the composition of spreading and interpolation yields the identity. Starting from any Lagrangian variable, \( \phi_p \): spread gives \( \phi^S_i = \sum_p \phi_p \delta^S_{ip} \) and interpolation \( \phi^{SI}_p = \sum_q \sum_i \delta^I_{ip} \delta^S_{iq} \phi_q \). Therefore \( \phi^{SI}_p = \phi_p \) if

\[
\sum_i \delta^I_{ip} \delta^S_{iq} = \delta^kr_{pq}
\]

Where \( \delta^kr_{pq} \) is the Kronecker delta. As discussed by Peskin [7], the kernels satisfy a softer property, namely \( \sum_i \delta^I_{ip} \delta^S_{ip} = 1 \) However, as they only differ from zero within a finite width (2h in our implementation), in practice, Eq. (16) strictly holds if particles cannot not overlap. This can be ensured either by lubrication or (steric) repulsive interparticle potentials.

3.2 Integration

The particle and fluid equations of motion will be integrated using a time step \( \Delta t \). The discrete set of times is noted as \( t_n = n \Delta t \). We now follow the sequence of steps of the
algorithm hereby derived although for now, we keep time integrals by introducing this notation,
\[ \bar{\phi} \equiv \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \phi(t)dt \] (17)

• Following the same line leading to Eqs. (10) and (11), the first step of the algorithm derives the unperturbed Eulerian velocity,
\[ \rho \tilde{u}_i = \rho u^n_i - [\nabla \cdot \Pi]_i \Delta t \] (18)

where \( u^n_i = u(r_i, t_n) \), etc.

• The Eulerian unperturbed velocity is interpolated at the Lagrangian sites \( p = \{1, ..., M\} \). It is important to note that the interpolator and spreading operators depend on time via the particle position. We shall indicate this dependence in the particle subscript, e.g. \( \delta^I_{ip} = \delta^I(|r_i - R_p(t_n)|) \). The updated particle positions \( R^{n+1}_p = R^n_p + \bar{V}_p \Delta t \) are used to evaluate the interpolated unperturbed velocity
\[ \tilde{u}_p = \sum_i \delta^I_{ipn+1} \tilde{u}_i \] (19)

• The updated particle velocity is obtained upon integration of Eq. (9) where the fluid-particle force in turn depends on the particle velocity. However Eq. (12) introduces the integrated effect of this force instantaneously at the end of the integration step (time \( t_{n+1} \)). This fact and the assumption of non-overlapping kernels simplify the (otherwise transcendental) equation (9) and (12) to a linear system for \( V_p \) and \( F_p \) which can be solved in a single step (i.e. without costly iterations). The updated particle velocity results,
\[ V^{n+1}_p = V^n_p + \frac{m_p}{\Delta M_p + m_p} (\bar{u}_p - V^n_p) + \frac{\bar{F}_{\text{ext}} \Delta t}{\Delta M_p + m_p} \] (20)
The fluid mass within the particle domain is denoted as \( m_p = \rho V_p \sum_i \delta^I_{ip} \); for an incompressible fluid \( m_p = \rho V_p \).

• The particle-fluid force is now spread to the Eulerian nodes. As before, the volume integral over one fluid cell of volume \( h^3 \) is \( \int_{h^3} f(r)dr^3 \simeq f_i h^3 \). So from Eq. (7) the net gain in fluid momentum due to the particle presence is,
\[ \sum_i \int_{t_n}^{t_{n+1}} f_i dt' h^3 = \sum_p \int_{t_n}^{t_{n+1}} F_p dt' \] (21)
Equation (21) provides consistency between the interpolated Lagrangian forces and the Eulerian momentum gain (the consistency between spread Eulerian forces and
the Lagrangian momentum gain is discussed in next Section). The spreading operation should therefore ensure fulfillment of Eq. (21). To that end, the net momentum gain in the fluid due to the immersed particles is decomposed in individual particle contributions (i.e. \( f_i = \sum_p f_{ip} \)). Following Eqs. (7) and (12) leads to,

\[
\int_{t_n}^{t_{n+1}} f_p(t') \, dt' = \rho \left[ V_p^{n+1} - \tilde{u}_p \right] \delta S_{ip}^{n+1}
\]

which satisfies Eq. (21) provided that the spreading property (15) holds. One can finally add the particle’s spread momentum given by Eq. (22) to the unperturbed fluid momentum of each node “i” to get

\[
u_i^{n+1} = \tilde{u}_i + \sum_p \left( V_p^{n+1} - \tilde{u}_p \right) \delta S_{ip}^{n+1}
\]

An important test of the scheme is to ensure that the fluid velocity at Lagrangian site \( p \) obtained by interpolation of Eq. (23) yields the desired particle value. Multiplying Eq. (23) by \( \delta I_{ip}^{n+1} \) and summing over \( i \) leads to, \( \nu_p = \tilde{u}_p + \sum_q \left( V_q^{n+1} - \tilde{u}_q \right) \sum_i \delta I_{ip} \delta S_{iq} \). Thus \( \nu_p = V_p \) is satisfied provided that the already highlighted Eq. (16) holds.

4 Consistency: compressible fluids at Low Mach number

In this section we analyze the consistency between Eulerian and Lagrangian force-momentum conversion. To illustrate this point we consider a more general case: particles immersed in a compressible fluid. As an outcome we prove that a trivial modification of the present scheme [whereby the uniform density \( \rho \) is substituted by node values \( \rho_i \), in Eqs. (18) and (22)] is perfectly valid under low Mach number. This fact was confirmed in simulations.

The consistency one would like to achieve in the discretized scheme builds up from the local character of the fluid-particle force field \( f \) reflected in Eq. (6). This relation implies that the gain in fluid momentum due the particles presence can be equally obtained either by integrating over the whole fluid domain or by integration over the set of non-overlapping particle volumes \( \bigcup V_p \). For consistency, these two integrals should be equal in the numerical scheme: while the first integral (over the whole volume) is carried out with Eulerian variables, the second one (over particle volumes) corresponds to Lagrangian counterparts. To begin with, the fluid momentum introduced at one Eulerian node “i” by the particles over \( \Delta t \) is,

\[
h^3 \left( \Delta g_i + [\nabla \cdot \Pi]_i \Delta t \right) = \sum_p h^3 \mathbf{T}_{ip} \Delta t
\]

The total momentum gain is obtained by integrating over the whole domain. Its discretized Eulerian version is \( \Delta \mathbf{W}_E = h^3 \sum_i \left( \Delta g_i + [\nabla \cdot \Pi]_i \Delta t \right) \) where,

\[
\Delta \mathbf{W}_E = \sum_i \sum_p h^3 \mathbf{T}_{ip} \Delta t = \sum_p \mathbf{F}_p \Delta t
\]
The second equality is just Eq. (21) which, as stated, is guaranteed by the spreading property (15).

Before performing the force integral over the set of particle volumes, let us trivially generalize the spread force in Eq. (22) to a compressible density field, \( \{ \rho_i \} \):

\[
\overline{F}_{ip} \Delta t = \rho_i [ \overline{V}_p - \overline{u}_p ] \delta_{ip}^S.
\] (26)

Now, as stated above, in the point particle approximation the integral over the particle volume \( \int_{V_p} \phi(\mathbf{r}) d\mathbf{r}^3 \) is given by \( \phi_p V_p \), where \( \phi_p \) is a (interpolated) Lagrangian variable. To obtain the Lagrangian expression for the change of fluid momentum due to the particle \( p \) we interpolate of Eq. (24) at \( \mathbf{R}_p(t + \Delta t) \), add and extract \( g_p^n \) to get,

\[
\Delta g_p + [ \nabla \cdot \overline{\Pi} ]_{p_{n+1}} \Delta t = (g^n_{p_{n+1}} - g^n_p) + \nabla^{-1} F^p_p \Delta t
\] (27)

Where we have introduced the notation \( g^n_{p_{n+1}} = \sum_i g^n_i \delta_{ip} \) to express a Eulerian field at time \( t_n \) interpolated at the particle position \( \mathbf{R}_p(t_n + \Delta t) \) in the updated time. Whenever both times coincides we simplify the notation, \( g^n_{p_{n+1}} = g^n_{p_{n}} \) and indeed \( \Delta g_p = g^n_{p_{n+1}} - g^n_p \).

The modified particle force appearing in Eq. (27) arises from the force density chosen in Eq. (26), \( \nabla^{-1} F^p_p \Delta t = \sum_i \overline{r}_{ip} \delta_{ip} \), resulting in

\[
\overline{F}^p_p \Delta t = \nabla^{-1} \rho_p \left[ V^p_{p_{n+1}} - \overline{u}_p \right] \quad \text{with}
\]

\[
\rho_p^s = \sum_i \rho_i \delta_{ip} \delta_{ip}^S
\] (29)

Before dealing with this force, let us first analyze the new convective term appearing in Eq. (27). Introducing the Lagrangian spatial derivative \( \nabla_R \phi \cdot d\mathbf{R} = \phi(\mathbf{R} + d\mathbf{R}) - \phi(\mathbf{R}) \) leads to,

\[
g^n_{p_{n+1}} - g^n_p = \nabla_R g^n_p \cdot V_p \Delta t = \left( \nabla \cdot [g^n_p V_p] - \overline{V}_p \nabla_R \cdot g^n_p \right) \Delta t
\] (30)

For an incompressible fluid \( \partial_t \rho_p = -\nabla \cdot g_p = 0 \) and the second term vanishes. In the compressible case it is not difficult to see that the last term of Eq. (30) simplifies out \(^1\)

Extracting the convective term from the stress tensor \( \overline{\Pi} = \mathbf{gu} + \mathcal{P} \) leads to

\[
\Delta g_p + \nabla_R \cdot \mathcal{P}^n_{p_{n+1}} \Delta t = \nabla_R \cdot \left( g^n_p V_p - \overline{gu}_p \right) \Delta t + \overline{F}^p_p \nabla^{-1} \Delta t
\] (31)

where we have used that \( \nabla \cdot \phi^p_p = \nabla_R \cdot \phi_p \) \(^2\) and also used that \( \mathcal{P} \) is linear. Alternatively, by also adding and extracting \( \left[ \nabla \cdot \overline{\Pi} \right]_{p_{n+1}} \Delta t \) to Eq. (27) leads to,

\[
\Delta g_p + \nabla_R \cdot \mathcal{P}^n_{p_{n+1}} \Delta t = \nabla_R \cdot \left( g^n_p V_p - \overline{gu}_p \right) + \overline{F}^p_p \nabla^{-1} \Delta t
\] (32)

\(^1\)To see this one can decompose \( \phi_i = \phi_p + \delta \phi_i \) (so that \( \delta \phi_p = 0 \) by construction). Then in the LHS of Eq. (31) \( \Delta g_p = g^n_{p_{n+1}} - g^n_p = u^n_p [ \delta \rho_p + \rho^n_{p_{n+1}} \Delta u_p + \Delta \delta \rho u_p ] \). For the explicit scheme we are using \( \Delta \rho_p = -\nabla_R \cdot g^n_p \Delta t \) and \( \overline{V}_p = V^n_p = u^n_p \). Therefore the last term at RHS of Eq. (30) simplifies out, but still one is left with a momentum contribution due to the convection of density-velocity correlations inside the kernel.

\(^2\)This comes from the fact that the interpolator only depends on distances \( |\mathbf{r} - \mathbf{R}| \), so the interpolation of a shifted function is just \( \sum_i \phi(x_i + dx) \delta^p ([x_i - X]) = \sum_i \phi(x_i + dx) \delta^p ([|x_i + dx - (X + dx)|] = \phi^p (X + dx).
At this point it is instructive to consider \( F_p^* = 0 \), i.e., no particle in the fluid. In this case Eq. (31) should ideally provide the Lagrangian motion of a fluid parcel determined by the material derivative \( \rho Du/ Dt = -\nabla R_p P \). One finds however that the convective terms in the right hand side (RHS) of Eq. (31) do not exactly cancel out for two reasons. The first is unavoidable and comes out from the finite width of the kernels used. In other words \( \phi_p = \phi^n_p + [\delta g/\delta u]_p \) so (the divergence of) momentum-velocity correlations inside the kernel domain contribute in the “parcel” equation of motion. The second source of error comes from the different momentum field encountered by the particle before and after each jump in position, during its discrete time integration. For our explicit scheme \( \phi_p = \phi^n_p \) the RHS of Eq. (31) becomes \( 3 \) of order \( \rho u^3 \Delta t^2/ h^2 \) and it is smaller than the viscous term on the LHS (\( \rho u \Delta t/ h^2 \)) if \( \text{Re} = uh/ \nu < 1/ C \) where \( C = u \Delta t/ h \) is the Courant number \( C < 1 \).

Expressing the momentum balance in the form of Eq. (32) more clearly indicates that this term is the momentum convected by the particle in space and time (indeed it contains the memory of the particle induced forces).

In conclusion the scheme yields the following total momentum change from the Lagrangian variables,

\[
\Delta W_L = \sum_p F_p^* \Delta t + O(\rho u^3 \Delta t^2/ h^2) \tag{33}
\]

Equation (33) with (28) and (29), is the Lagrangian version of the Eulerian momentum balance in Eq. (25). Up to the \( O(\Delta t^2) \) difference, whenever \( F_p^* \neq F_p \), some inconsistency is introduced in the Eulerian-Lagrangian force transformation. In the incompressible formulation \( \rho_p = \rho \), Eq. (29) ensures consistency between the Eulerian and Lagrangian total momentum \( \Delta W_E = \Delta W_L \) provided the celebrated condition (16) holds.

Any inconsistency in the Lagrangian momentum balance will affect the meaning of the particle “mass” because it can only be dynamically understood (force/acceleration). Fortunately, the property (16) tell us that \( \delta \rho_p \delta \phi_p \) is also an interpolator which satisfies (14) so one should expect \( \rho_p \simeq \rho_p^n \) and \( F_p^* \simeq F_p \). One can always write, \( F_p^* = F_p + (m_p^* - m_p) \alpha_p \delta \), where \( \alpha_p \Delta t = V_p - \bar{u} \). The fluid mass “inside” the particle are \( m_p = \rho_p V_p \) and \( m_p^* = \rho_p^* V_p \). It can be shown that this force difference \( \delta F = (m_p^* - m_p) \alpha_p \) satisfies \( \delta F / F < \delta \rho^{\text{max}} / \rho_p \sim Ma^2 \), where \( \delta \rho^{\text{max}} \) is the maximum density disturbance and Ma is the Mach number. In other words the scheme modified according to Eq. (26 is valid in the low Mach regime. Alternative implementation allowing arbitrary Mach and this will be presented elsewhere.

5 Results

We have performed a series of simulations to check the behavior of the present scheme. The first task consisted on measuring the hydrodynamic radius of the particle. As also happens in other Eulerian-Lagrangian solvers for point-wise particles (based on Stokes
coupling) [2], the hydrodynamic radius of the particle is determined by the width of the kernel, which in turns is proportional to the mesh size. The evaluation of the hydrodynamic radius is done by performing momentum conserving simulations of settling [2]. For a scheme based on the Stokes drag coupling \( \mathbf{F}_p = \xi_{\text{bare}} (\mathbf{V}_p - \mathbf{u}_p) \), one gets \( \frac{1}{R_H} = 1/a_0 + 1/gh + 2.84/L + O(L^3) \) where \( L \) is the periodic box size. The effective friction coefficient is thus the sum of the bare (input) friction \( (a_0 = \xi_{\text{bare}}/(6\pi \eta)) \) and that arising from the hydrodynamic field \( (gh = \xi_{\text{hydro}}/(6\pi \eta)) \). The DF approach instantaneously transfer the particle-fluid momentum; corresponding to \( \xi_{\text{bare}} = \infty \). This is indeed what we observe when plotting \( R_H \) against \( L \). We get \( g = 0.89 \) and the translational invariance of \( g \) is satisfied up to 1%.

The second set of simulations were carried out to analyze the drag force to a particle up to moderate Reynolds number \( Re < 10 \). Results for the drag force are compatible with those obtained by Padding and Louis [9] resolving solid 3D particles in a Stochastic Rotation Dynamics solver with slip boundary conditions at the particle surface. This result is consistent with the point-wise character of the model; whereby the fluid obviously slips at the (non-resolved) particle “surface”.

Velocity profiles around the particle at low Reynolds number were found to perfectly match the theoretical results. In order to avoid finite size effects we solved the (\( \text{Re}=0 \) limit) flow around a fixed sphere in a fluid with fixed velocity at distances \( \mathbf{R}_L \) from the sphere center.

Another test was to reproduce the hydrodynamic force between to particles as a function of their relative distance. Under low Reynolds and distances somewhat larger than the particle diameter this force is described by the Oseen expression [2]; while as they come closer lubrication forces become important and eventually diverge at contact. The DF point particle scheme correctly reproduces Oseen forces and is able to trace the initial force increase due to lubrication, when the particle centers are about 1.5 diameters apart.

Quite interestingly, the instantaneous transfer of momentum between fluid and particle ensures that there is no extra dissipative channel in the particle motion (as occurs in Stokes coupling [2]). This means that the particle kinetic temperature thermalizes with the fluid and its velocity follows a Boltzmann distribution at the fluid temperature, without the need of extra noise terms in the particle motion. Under fluctuating hydrodynamics we have also checked that the time correlation of the particle velocity properly recovers the long-time algebraic tail \( ((\nu t)^{3/2}) \) [9]. Finally simulations for an array of particles under the presence of a stationary plane sound wave of frequency \( \omega \) were performed to measure the acoustic force on the particles. Comparison was made with the theory developed by Gor’kov [3]. Three length scales govern this problem: the acoustic boundary layer \( \delta = \sqrt{\nu/\omega} \) (with \( \nu = \eta/\rho \)) the wavelength \( \lambda = c 2\pi/\omega \) and the particle particle radius \( R \). Simulations were performed for a small particle \( (R_H/\lambda \simeq 0.044) \) in the non-viscous regime \( (\delta/R_h \simeq 0.27) \). It is noted that Stokes coupling is only valid for \( \delta/R_H >> 1 \). The radius of the particle and the sound velocity across the particle \( c_p \) are the two only adjustable parameters. We found that simulations perfectly fit the theoretical prediction
if $R = 1.2 R_H$ and $c_p = c_f$, where the solvent sound velocity $c_f$ corresponds to water at $T = 300K$ [8]. Density perturbations were kept at low Mach, according to the predicted limitation of the present formulation (see above).

In summary we have presented an extension of Direct Forcing in Eulerian-Lagrangian schemes which can solve inertial effects on the particle and it is naturally adapted to fluctuating hydrodynamics. The algorithm is quite easy to adapt from a Stokes coupling algorithm and can be used to solve low Mach number flows up to moderate particle Reynolds number $Re < 10$. Future extension for arbitrary Ma and larger Re are underway. With these generalizations we expect this method to have an impact in the study of finite particle size effects in turbulent flows.

REFERENCES


SIMULATING THE DYNAMIC BEHAVIOR OF DROPLET IN A GROOVED CHANNEL BY DISSIPATIVE PARTICLE DYNAMICS

M. K. ZHANG*, S. CHEN*# AND Z. SHANG†

* School of Aerospace Engineering and Applied Mechanics
Tongji University
Siping Road No. 1239, 200092 Shanghai, P. R. China

#corresponding author, e-mail: schen_tju@mail.tongji.edu.cn

† Science and Technology Facilities Council
Daresbury Laboratory
Warrington WA4 4AD, UK

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Abstract. In this paper, an improved dissipative particle dynamics (DPD) method was applied to simulate droplet motion in a grooved microchannel. Firstly the static contact angle between the droplet and the solid wall was simulated with the improved potential function, and "static contact angle~a_{wf}/a_f" curve was obtained by Polynomial Fit of the 2nd order. Then the influences of wall wettability, flow field force on the flow pattern of droplet were investigated in a grooved microchannel. The results show that wall wettability and flow field force have large effects on the flow pattern of the droplet.

1 INTRODUCTION

In the past decade, a variety of concepts has been developed for the construction of microfluidic system. For example, Yun et al.[1] proposed a micropump actuated by surface tension based on continuous electrowetting, this kind of micropump has achieved comparable performance to previous micropumps operated by various actuation mechanisms with extremely low power consumption and low voltage operation and can be used in application fields such as handheld micro lab-on-a-chips and portable biomedical devices where large pump pressure is not required. Gordillo et al. [2] presented a new method for the production of bubble-liquid suspensions composed of micro-sized bubbles. Using computer simulations, Kuksenok et al. [3] investigated the behavior of an immiscible binary AB fluid that is driven to flow through a microchannel, which is decorated with a checkerboard pattern of chemically distinct A- and B-like patches on the top and bottom walls. The results provided guidelines for designing microfluidic devices that can be used to effectively intermix multicomponent fluids. The development of microfluidic system usually requires understanding the mechanism of fluid flows, involving in various wetting, capillary phenomenon and fluid flow behaviors with free surfaces.

Many researches have demonstrated that roughness may apparently increase the hydrophobicity or hydrophilicity of the surface. Seemann et al.[4] reported even relatively
simple surface topographies such as grooves with rectangular cross section exhibit a large variety of different wetting morphologies. Mchale et al. [5] investigated topography driven spreading. Their results showed roughening a hydrophobic surface enhances its nonwetting properties into superhydrophobicity, and topographic effects can also enhance partial wetting by a given liquid into complete wetting to create superwetting. Huang et al. [6] studied a droplet moving inside a grooved channel by using a new lattice Boltzmann model for multiphase flows with large density ratio. The impacts of the adhesion and geometrical properties of the surface on the flow pattern and droplet velocity have been explored in detail.

The purpose of the present study is to obtain numerical simulation results for droplet motion in a grooved channel by dissipative particle dynamics. A modified particle-particle interaction potential with a combination of short-range repulsive and long-range attractive interaction is adopted to achieve vapor-liquid coexistence, and it could be used to simulate the flow behaviors of fluid with free surfaces. The effects of wall wettabiliy and flow field force on the flow pattern of the droplet in a grooved microchannel have been discussed.

2 DISSIPATIVE PARTICLE DYNAMICS AND ITS MODIFICATION

Dissipative particle dynamics (DPD) is a mesoscale fluid simulation method proposed by Hoogerbrugge and Koelman [7]. The DPD model consists of particles representing molecular clusters, interacting with each other via conservative, dissipative, and random forces. Because the interaction between clusters of molecules is much softer than molecule-molecule interaction, longer time steps than MD could be taken in DPD.

In DPD system, the motion of each particle having position \( r_i \) and velocity \( v_i \) is governed by the kinematic theory \( \frac{d r_i}{d t} = v_i \) and Newton’s second law \( \frac{d v_i}{d t} = F_i \), here the mass of each particle is taken as unit. Besides external force, the force \( F_i \) could be decomposed into conservative, dissipative and random components:

\[
F_i = \sum_{j \neq i}(F_{c,ij} + F_{d,ij} + F_{r,ij})
\]

In formula (1), the distance between the two particles determines the magnitude of the conservative force \( F_{c,ij} \). The dissipative component \( F_{d,ij} \) is used to model viscosity of fluids while the random one \( F_{r,ij} \) compensates the kinetic energy reduced by dissipative force.

The conservative force usually takes the form:

\[
F_{c,ij} = a_{ij} w_c(r_{ij}) \hat{r}_{ij}
\]

where \( w_c(r_{ij}) \) is the weight function; \( a_{ij} \) is the interaction strength, which is the main parameter that models the local hydrostatic pressure in fluids; \( r_{ij} = |r_i - r_j| \), \( r_i = |r_i| \), and \( \hat{r}_{ij} = r_{ij}/|r_{ij}| \).

In conventional DPD, the conservative force weight function is a pure repulsive function:

\[
w_c(r_{ij}) = (1 - r_{ij}/r_c)
\]

here \( r_c \) is the cutoff radius, meaning that \( w_c(r_{ij}) \) vanishes for \( r > r_c \). For more details, please see reference [8]. Conventional DPD particles interact with each other via soft interaction, leading to the apparent absence of a \( \rho^3 \) term in the equation of state, which can’t produce vapor-liquid coexistence [9]. To deal with this difficulty, Pagonabarraga and Frenkel [10] developed a multibody DPD (MDPD), in which the conservative interaction depends on the
instantaneous local particle density. Using MDPD model or its modified versions, Warren [11,12] and Tiwari [13] et al. simulated kinds of phenomena such as vapor-liquid interface, oscillation of a cylindrical drop etc. Liu [14,15] introduced a new method with a combination of short range repulsive and long range attractive interaction to explore the potential of simulating the vapor-liquid coexistence and free surface phenomena.

In order to simulate the vapor-liquid coexistence or flow phenomena of liquids with free surface, in the present study the combination of short range repulsive and long range attractive interaction proposed by Liu [14,15] was applied to modify the conservative force, i.e. purely repulsive interaction, of the conventional DPD model. This new interaction potential is constructed by a linear combination of cubic spline which is often used in smoothed particle hydrodynamics (SPH), with different cutoff radius. The most commonly used smoothing function in SPH [16] is the cubic spline:

\[
W(r) = W(r, r_c) = \begin{cases} 
1 - \frac{3}{2} \left( \frac{2r}{r_c} \right)^2 + \frac{3}{4} \left( \frac{2r}{r_c} \right)^3 & 0 \leq \frac{2r}{r_c} < 1 \\
\frac{1}{4} \left[ 2 - \left( \frac{2r}{r_c} \right) \right]^3 & 1 \leq \frac{2r}{r_c} < 2 \\
0 & \frac{2r}{r_c} \geq 2 
\end{cases}
\] (4)

Our new interaction potential takes the form:

\[
U(r) = a[AW(r, r_{c1}) - BW(r, r_{c2})]
\] (5)

here \(W(r, r_{c1}), W(r, r_{c2})\) are cubic splines; \(r_{c1}, r_{c2}\) are different cutoff radius; \(A\) and \(B\) are coefficients which could be adjusted simply to modify different long range attractive interaction; \(a\) is the interaction strength. The DPD conservative force is obtained by taking the gradient of the new potential:

\[
F_{C,ij} = -\frac{dU(r)}{dr} \hat{F}_{ij} = -a[AW'(r, r_{c1}) - BW'(r, r_{c2})] \hat{F}_{ij}
\] (6)

For the choice of parameters, one case of interaction potential frequently used in this paper is:

\[
U(r) = 18.75[2.0W(r, 0.8) - W(r, 1.0)]
\] (7)

which could achieve liquid-gas density ratio larger than 600, and could be used to approximately simulate the flow flows with free surfaces [14].

3 RESULTS AND DISCUSSION

3.1 Simulation of static contact angle

The solid wall is represented by using frozen particles in the present study. Near the wall a thin layer is assumed where the no-slip boundary condition holds. A random velocity distribution is enforced in this layer with zero mean corresponding to a given temperature. Similar to the reflection law of Revenga et al. [17], we further require that particles in this layer always leave the wall. The velocity of particle \(i\) in the layer is

\[
\mathbf{v}_i = \mathbf{v}_R + \mathbf{n}(\sqrt{(\mathbf{n} \cdot \mathbf{v}_R)^2 - \mathbf{n} \cdot \mathbf{v}_R})
\] (8)

where \(\mathbf{v}_R\) is the reandom vector and \(\mathbf{n}\) is the unit vector normal to the wall and pointing to the fluid. For more details, please see reference [18].

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The wettability could be adjusted from hydrophobicity to hydrophilicity by changing the ratio of \( \frac{a_{wf}}{a_f} \). Fig. 1 shows three different cases, in which the static contact angle is from 103° to 54°. With the increase of ratio \( \frac{a_{wf}}{a_f} \), the attractive force between the wall particles and the fluid particles is strengthened, the static contact angle becomes smaller.

\[
\theta = 20.202\left(\frac{a_{wf}}{a_f}\right)^2 - 129.71\left(\frac{a_{wf}}{a_f}\right) + 181.61
\]

Accordingly, the relation curve between \( \frac{a_{wf}}{a_f} \) and static contact angle is shown in Figure 2.

3.2 Simulation of droplets motion in grooved microchannel

3.2.1 Effect of wall wettability

The computational domain consists of three phases: droplet, vapor and solid wall of the channel, as shown in Fig. 3. The lower wall of the channel is roughened by grooves. The size of the channel is 120 × 10 × 16, while the size of the grooves is set as 7 × 3 and the size of the protuberant part is 3 × 3. There are totally 37760 DPD particles in the computational domain, in which the wall and the fluid are made up of 16960 and 20800 particles, respectively. The initial configurations of fluid and wall particles are generated by a pre-processing program and read in as input data. The initial velocities of the fluid particle are set.
randomly according to the given temperature, while the wall particles are frozen. Periodic boundary conditions are applied on the flow boundaries of the computational domain in the X and Y directions.

From the Polynomial Fitting curve as shown in Fig. 2 we can see that the static contact angles of 130°, 110°, 90°, 70° and 50° correspond to the ratios of $a_{uL}/a_f$ from 0.426, 0.610, 0.808, 1.024 to 1.263, respectively, Similar to reference [6]. The upper wall is kept neutral-wetting (i.e. $\theta = 90^\circ$), while the lower contact angles are adjusted from hydrophobicity to hydrophilicity.

Using the improved weight function, vapor-liquid coexistence could be reached. The parameters $a$, $A$, $r_{x1}$, $r_{c2}$ are set as in Equation (7), so liquid-gas density ratio of larger than 600 could be obtained [14]. At the beginning of the simulation the particles are allowed to move without applying the external force until the thermodynamic equilibrium state is reached. Then the external force field of $g = 0.01\sqrt{\dot{z}}$, $\alpha_f = -45^\circ$ is applied to fluid particles and the nonequilibrium simulation starts. Fig. 5 shows the snapshots of the droplet motion under different wettability. With the increase of the hydrophilicity, the drag acted on the droplet increases, the flow velocity of the droplet becomes smaller, which is in agreement with the simulation results of reference [6] by LB method.

![Figure 5: Snapshots of the droplet motion under different wettability](image)

Fig. 6 shows the comparison of droplet motion velocity under different wetting conditions. The droplet repeats the motion mode of “contact with one protuberant part” and “contact with two protuberant parts”. When the droplet contacts with one protuberant part, the contact area decreases, and the drag force decreases. Accordingly, the droplet velocity increases. While the droplet contacts with two protuberant parts, the contact area increases, and the drag force increases. Accordingly, the droplet velocity decreased. Hence it is noted that velocity fluctuation exists when the droplet move forward from Fig 6.
randomly according to the given temperature, while the wall particles are frozen. Periodic boundary conditions are applied on the flow boundaries of the computational domain in the X and Y directions.

From the Polynomial Fitting curve as shown in Fig. 2 we can see that the static contact angles of 130°, 110°, 90°, 70° and 50° correspond to the ratios of from 0.426, 0.610, 0.808, 1.024 to 1.263, respectively, Similar to reference [6]. The upper wall is kept neutral-wetting (i.e.), while the lower contact angles are adjusted from hydrophobicity to hydrophobicity. Using the improved weight function, vapor-liquid coexistence could be reached. The parameters , are set as in Equation (7), so liquid-gas density ratio of larger than 600 could be obtained [14]. At the beginning of the simulation the particles are allowed to move without applying the external force until the thermodynamic equilibrium state is reached. Then the external force field of is applied to fluid particles and the nonequilibrium simulation starts. Fig. 5 shows the snapshots of the droplet motion under different wettability. With the increase of the hydrophobicity, the drag acted on the droplet increases, the flow velocity of the droplet becomes smaller, which is in agreement with the simulation results of reference [6] by LB method.

![Figure 5: Snapshots of the droplet motion under different wettability](image)

Fig. 6 shows the comparison of droplet motion velocity under different wetting conditions. The droplet repeats the motion mode of "contact with one protuberant part" and "contact with two protuberant parts". When the droplet contacts with one protuberant part, the contact area decreases, and the drag force decreases. Accordingly, the droplet velocity increases. While the droplet contacts with two protuberant parts, the contact area increases, and the drag force increases. Accordingly, the droplet velocity decreased. Hence it is noted that velocity fluctuation exists when the droplet move forward from Fig 6.

![Figure 6: Comparison of droplet velocity under different wetting conditions](image)

**3.2.2 Effects of external force direction**

In this section, the effects of external force direction on the droplet motion are investigated by keeping the horizontal component of external force fixed and changing the vertical component. The upper and lower walls are kept neutral wetting, two kinds of external force directions are applied: ① and ② . Fig. 7 shows the different dynamic behaviors of droplet motion in flat plate channel under different external force directions.

![Figure 7: Comparison of droplet motion under different external force directions](image)

Then we simulate the dynamic behaviors of droplet in grooved channels. Three kinds of external force directions are applied: ① ② , and ③ . Fig. 8 shows comparison of snapshots of droplet motion under different external force directions. As can be seen from Fig. 8, the contact area between the droplet and the protuberant parts of the lower wall increases with the increase of . The smaller the downward component of field force is, the faster the droplet flows in the microchannel.
Fig. 8: Comparison of snapshots of droplet motion under different external force directions

Fig. 9 shows the comparison of droplet velocity under different external force directions. The vertical component of external force enhances the contact of the droplet on the wall, hence the velocity fluctuation of the droplet is enlarged when the vertical component is increased.

Fig. 9: Comparison of droplet velocity under different external force directions

4 CONCLUSIONS

In the present study, a modified DPD method with a combination of short-range repulsive and long-range attractive interaction is adopted to investigate the dynamic behaviors of droplet in a grooved channel. The results show that the wettability of wall and external force direction significantly affect the dynamic behaviors of droplet in grooved channel. The motion velocity of the droplet decreased with the increase of the wettability. There exists velocity fluctuations when the droplets move inside a grooved channel, and the magnitude of the velocity fluctuations is related to the wetting conditions and the vertical component of the external force. This study is helpful to understand the fluid flow behavior with free surface on rough surfaces.
REFERENCES


Abstract. This paper outlines the problems found in the parallelization of SPH (Smoothed Particle Hydrodynamics) algorithms using Graphics Processing Units. Different results of some parallel GPU implementations in terms of the speed-up and the scalability compared to the CPU sequential codes are shown. The most problematic stage in the GPU-SPH algorithms is the one responsible for locating neighboring particles and building the vectors where this information is stored, since these specific algorithms raise many difficulties for a data-level parallelization. Because of the fact that the neighbor location using linked lists does not show enough data-level parallelism, two new approaches have been proposed to minimize bank conflicts in the writing and subsequent reading of the neighbor lists. The first strategy proposes an efficient coordination between CPU-GPU, using GPU algorithms for those stages that allow a straightforward parallelization, and sequential CPU algorithms for those instructions that involve some kind of vector reduction. This coordination provides a relatively orderly reading of the neighbor lists in the interactions stage, achieving a speed-up factor of x47 in this stage. However, since the construction of the neighbor lists is quite expensive, it is achieved an overall speed-up of x41. The second strategy seeks to maximize the use of the GPU in the neighbor’s location process by executing a specific vector sorting algorithm that allows some data-level parallelism. Although this strategy has succeeded in improving the speed-up on the stage of neighboring location, the global speed-up on the interactions stage falls, due to inefficient reading of the neighbor vectors. Some changes to these strategies are proposed, aimed at maximizing the computational load of the GPU and using the GPU texture-units, in order to reach the maximum speed-up for such codes. Different practical applications have been added to the mentioned GPU codes. First, the classical dam-break problem is studied. Second, the wave impact of the sloshing fluid contained in LNG vessel tanks is also simulated as a practical example of particle methods.
1 INTRODUCTION

The recent implantation of graphic process units (GPUs) in scientific computation has increased drastically the speed processing in several applications. Not many years ago, parallel computing was restricted to super-computing centers or large and expensive clusters. Nowadays, thanks to the arrival of GPU multicore processors, originally designed for graphic processing, massively parallel processing is becoming increasingly more accessible and cheaper for the developer.

Increasing the efficiency of algorithms involved not only depends on the specific hardware improvements, but also on the new approaches aimed at maximizing available resources and minimizing costs. In the case of GPU processors, it is necessary to note that the computational power computer lies in its specialization. The GPU multicore architecture is designed for highly efficient graphic processing. This requires the implementation of affine and projective orthogonal transformations (matrix operations) on a set of elements (vertices, fragments) between different spaces of the 3D graphic scene. Likewise, the level of independence between these elements is perfect for parallel processing through which it is possible to distribute among a large number of processors such arithmetic operations on each of the vertices and fragments of the scene, commonly arranged as large vectors.

In order to exploit this powerful calculation, the GP-GPU emerges as a discipline where graphics shader functions are redesigned for processing data vectors, not necessarily graphics, which might exhibit a high level of parallelism from the point of view of SIMD (Single Instruction-Multiple Data) architectures.

To explore the degree of adaptability of the GPU technology to certain algorithms which simulate large particle systems, first we analyze which steps of the SPH (Smoothed Particle Hydrodynamics) code are more suitable to be parallelized, as well as different strategies of parallelization of the main subroutines. This requires the evaluation of the problematic aspects and the consequent speedup and scalability obtained.

Since the SPH methodology generally uses an explicit resolution scheme, their algorithms are easily parallelized on its minimum units (particles, cells). However, there are certain subroutines whose GPU parallelization is not immediate, in those cases different strategies will be implemented. These strategies will be focused on the obtention of the maximum parallelization implementation or the increase of the CPU versatility. Although it is always possible to use the CPU in those subroutines whose parallelization is problematic, this should be avoided due to the relatively high latencies associated with data transfers between CPU and GPU and the consequent reductions in computational performance.

2 GP-GPU: CUDA IMPLEMENTATION.

Traditionally, the GP-GPU has been developed using special languages (shaders) as GLSL, CG, or HLSL incorporated as extensions of the OpenGL and Direct3D APIs.
Learning GP-GPU programming not only required graphic programming as prerequisite, but also requires a considerable expertise on APIs and graphic languages. Currently, developing GP-GPU applications is done with the help of programming environments specifically designed to develop this type of codes as the CUDA (Computing Unified Device Architecture) or the OpenCL platforms.

2.1 Generalities.

Regarding GPU architecture, in Figure 1 a scheme of the distribution of the processors on the graphic cards used is shown. Basically, the GPU distributed in a set of multiprocessors. Each multiprocessor hosts typically 8 scalar processors in NVIDIA architectures. From the viewpoint of parallel codes, the first important concept to consider concerns the kernel functions (analogous to the shaders in the graphic computing context). When a kernel is called, throws a vector of N threads, each of which ends up being executed on a processor. In turn, every thread executes the instructions found in the kernel function sequentially. Once the kernel function is called, the N threads perform the instructions in parallel. Threads are grouped into blocks of threads. The ones associated in a specific block are executed in a common multiprocessor (8 single processors) where they can share variables and make use of the shared memory space associated with each multiprocessor.

When a kernel is called, blocks of threads are listed and distributed in the multiprocessors available. The threads of a block are executed simultaneously on a single multiprocessor, while multiple blocks could be executed concurrently in one multiprocessor. When all the threads of a block have finished, new blocks are launched in the vacant multiprocessors.

One multiprocessor can execute hundreds of threads concurrently. To manage this large number of threads, it uses a special architecture called SIMT (Single Instruction, Multiple Thread). This amount of threads are grouped into 32 unit packs called warps. In the SIMT architecture, the threads of a warp execute the same kernel instruction at the same time. Each multiprocessor is constantly alternating between warps, which can

Figure 1: Basic architecture of a GPU card.
decrease the latencies associated with the threads memory access and minimize the time when processors are inactive.

In order to make a parallel implementation, it is crucial to understand the GPU memory hierarchy to manage different memory spaces in order to achieve maximum transfer rates and avoid bottlenecks.

- **Registers**: Is a set of quick access memory banks used by the multiprocessors for local data allocation.

- **Shared memory**: Each multiprocessor has a shared reading and writing memory space only visible by the processors. This type of memory could be as quick as the registers, but the speed strongly depends on the way the code prevents access conflicts between processors.

- **Global memory**: is the read/write memory space visible for all GPU processors. This memory is relatively slow compared to reports the former ones. As the shared memory type, the amount of flow data depends on the way threads access to it.

- **Texture memory**: is a read only memory and can improve noticeably the performance if used properly.

### 2.2 High performance tips.

In [1] a series of essential strategies to obtain a maximum GPU performance are shown. Although following these guidelines is desirable, the implementation on the some of them depends on the nature of algorithm to parallelize.

- When consecutive half-warp threads read or write consecutive elements of a 32, 64 or 128 bytes memory segment of an array, the memory transfer of such items is done on a transaction, reaching huge memory transfer rates. Coalescent access to memory may occur either in the global memory or in the shared memory.

- Using shared memory to store those data that can be used by multiple threads of a block instead of global memory could achieve transfer rates 100 to 150 times higher.

- Minimize differences between threads of a warp is essential, because the SIMT architecture requires that warp threads are implicitly synchronized.

- Each multiprocessor is designed to manage hundreds of thread blocks and hundreds of thousands of threads simultaneously. As the number of processors is limited to 8, each multiprocessor is constantly alternating services among warps. When the occupation is very high, processors should not inactive waiting some threads to complete memory transactions, and they should give a temporary control to other threads from other warps that are ready to execute instructions. This decreases the latency associated to memory transfer efficiently.
3 SPH Parallel codes.

3.1 Introduction.

Smoothed particle hydrodynamics (SPH) is a Lagrangian method, with no computational mesh and has been widely employed to study free-surface flows. Originally invented for astrophysics during 1970s [7, 8], it has been applied to many different fields of the fluid dynamics and solid mechanics during the last decades. Instead of using a mesh, the SPH methods use a set of interpolation nodes placed arbitrarily within the fluid. This gives several advantages in comparison to mesh-based methods when simulating nonlinear flow phenomena. The method uses discrete approximations to interpolation integrals to change partial differential equations of fluid dynamics into summations. More complete reviews on standard SPH can be found at [9]. The SPH method is capable of dealing with free-surface problems, deformable boundaries, moving interfaces, wave propagation and solid simulation [2, 3]. In contrast, traditional numerical methods have difficulties to compute large deformations on the computational domain and also require special treatment (VOF, Level Set, etc...) to deal with free surface flows. Due to the large number of interactions for each particle at each time step, when SPH codes are computed on a single CPU they take a large computational time. When millions of particles are necessary to compute accurately a physical process, only parallel computing can guarantee efficient computational times. Graphics Processing Units (GPUs) thanks to their multi-threading capability can treat large data flows efficiently. Due to the inexorable development of the market of video games and multimedia, their computing power with streaming multi-processor technology has increased much faster than of CPUs. Thus, GPUs appear as an accessible alternative to accelerate SPH models using a powerful parallel programming model where the graphics cards are used as the execution devices. Their performance can be compared with large cluster machines. A huge advantage is the price and the easy maintenance GPUs need in comparison with large multi-core systems.

The capability of GPUs to handle with SPH was shown by the pioneer work of Harada [4], where they were able to simulate 60,000 particles in real time and they obtained runs over 28 times faster using a GPU than a CPU with tests of 260,000 particles. The method proposed was implemented using a GeForce 8800GTX GPU and developed before the appearance of CUDA, which means that Haradas work supposed a significant advance even when most of its limitations could be fixed using the advanced GPU programming features introduced by CUDA. Recent works concerning SPH computing on GPU can be found in [5].

3.2 Formulation.

In the SPH technique, the fluid domain is represented by a set of particles scattered in space where different physical properties are known (mass, density, pressure, position, velocity). These mesh-free particles move according to the governing fluid dynamics (Navier-Stokes) equations. The properties can change throughout a simulation due to the
interaction of neighboring points. Herein, the SPH formulation implemented on the GPU architecture is described briefly.

3.3 Interpolation.

As mentioned in the introduction, our goal is to simulate newtonian and incompressible viscous flow in laminar regime. These flows are well described in the continuous formulation by the Navier-Stokes equations:

\[
\nabla \cdot \mathbf{v} = 0 \\
\rho \frac{d\mathbf{v}}{dt} = -\nabla P + \mu \nabla^2 \mathbf{v}
\]

in which \( P \) is the pressure, \( \rho \) the density, \( \mathbf{v} \) the velocity and \( t \) stands for time.

Equation (1) and the pressure term in equation (2) play a combined role. The pressure acts as a Lagrange multiplier that produces a zero divergence velocity field. If the incompressibility condition is imposed, either a penalty formulation or a pressure Poisson equation must be solved to calculate the pressure values consequently increasing the computational cost substantially. In the WCSPH context this hypothesis is relaxed by assuming a weakly compressible fluid with a large sound speed, where the equation (1) is replaced by

\[
\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v}
\]

and a stiff equation of state \( P = P(\rho) \) is added to the system.

Finally, assuming the Lagrangian description of the fluid, the fluid particles move according to the kinematic law:

\[
\frac{d\mathbf{r}}{dt} = \mathbf{v}
\]

where \( \mathbf{r} \) is the position vector.

The interpolation method in SPH is based on the following integral:

\[
\langle f(\mathbf{r}) \rangle = \int_V f(\mathbf{r'}) W(\mathbf{r} - \mathbf{r'}, h) d^3 \mathbf{r'}
\]

where the integral extends over the domain \( V \), \( d^3 \mathbf{r'} \) is the element of volume dependant on the dimensions of the problem, \( \mathbf{r} \) and \( \mathbf{r'} \) are position vector and \( W(\mathbf{r} - \mathbf{r'}, h) \) is the interpolation or kernel function. The parameter \( h \) determines the size of the kernel, which means the distance of influence around \( \mathbf{r'} \). The integrals are replaced numerically by summations of the contributions of nearby particles.

The complete SPH formulation [9] considered will be the following:
\[
\frac{dp_a}{dt} = \sum_{b \in N_a} m_b \mathbf{v}_{ab} \nabla_a W_{ab} \\
\frac{dv_a}{dt} = -\sum_{b \in N_a} m_b \left( \frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla_a W_{ab} + \Pi_a
\]

\[P = \frac{\rho_0 c_s^2}{\gamma} \left( \frac{\rho}{\rho_0} \right)^\gamma - 1\]

in which \(m\) is the mass, \(\mathbf{r}\) is the position vector, and the subscripts \(a\) or \(b\) refers to the particle that carries over the considered property.

The notation \(\mathbf{v}_{ab}\) means \(\mathbf{v}_{ab} = \mathbf{v}_a - \mathbf{v}_b\), \(\nabla_a W_{ab}\) is the gradient of the \(b\)-centered kernel with respect to the coordinates of particle \(a\) and \(\Pi_a\) is the viscous term at particle \(a\) [9], \(N_a\) is the index set of particle \(a\) neighbors, regarding the kernel support, \(\rho_0\) the reference density, \(c_s\) is the numerical sound speed and \(\gamma = 7\).

The kernel used is a normalized Gaussian kernel, see [14], with a support of \(3h\) and \(h = 1.33 \, dx\) where \(h\) is the smoothing length and \(dx\) is the typical initial separation among particles.

The integration in time has been performed using a Leap-frog second order scheme[12]. The selection of the time step has been based on the viscous diffusion, convective, acceleration, and sound waves propagation terms[12]. The CFL factor used was 1/8 using \(h\) as a reference length. Depending on the case a special initialization or stabilization technique has been used.

Within SPH techniques, WCSPH is the usual way of modeling incompressible free surface flows [10, 15]. It is easy to programme because the pressure is obtained from a separate equation of state (8) that is chosen so that the speed of sound is large enough to keep the relative density fluctuations small [9]. However, when dealing with highly distorted flows the need for an explicit definition of a boundary at the free surface is a major drawback.

4 THE DAM-BREAK PROBLEM

We implemented the weakly compressible SPH method to simulate a 2D dam break problem with the geometric parameters shown in the figure 2. This geometric configuration is based on [6].

The walls of the tank are three particles thick and are modeled with boundary static particles, treated the same way as the fluid particles in the computation of the forces. At \(t = 0\) the fluid is completely still. The physical and numerical parameters were the following: \(h_{fac} = 1.33\), smoothing length \(h = 2.69 \cdot 10^{-2}\), initial distance between particles \(dx = h/h_{fac}\), reference density \(\rho_{ref} = 1000.0\), \(\gamma = 7.0\), numerical sound speed \(c_s = 15.0\), \(\alpha = 8\), dynamic viscosity \(\mu = 0.744\), gravity \(g = 9.81\) and Gaussian kernel type were used
in the simulation. For each particle $i$, the initial pressure has an hydrostatic distribution $p_i = \rho_{ref} \cdot g \cdot f \cdot (H - y_i)$ and the initial density is calculated according to equation (8).

4.1 CPU vs. GPU implementations

The table 1 shows the computational timings of seven executions corresponding to different values of the scale parameter $H$ and keeping constant the distance between particles $dx$. The smallest value of the scale parameter was $H = 0.6$. Due to the relatively high computational cost of the neighbor list construction stage in the parallel implementation, different GPU executions were done varying the frequency of the execution of this stage, so that the neighbor list construction is performed every $k$ steps of the algorithm in the GPU implementation.

In spite of the CPU sequential algorithm computes the neighbor list construction every step, this stage represents approximately 1% of the total computational time of the whole time step, consequently if the neighbor list construction were performed every $k$ steps the speed up factor would not be noticeably reduced in this implementation.

A maximum speed-up of $\times 41.5$ was obtained when 90079 particles were simulated. It should be noticed that the GPU implementation lacks of certain scalability when the algorithm deals with more than this amount of particles, possibly because in this GPU approach the CUDA kernels involved in the neighbor list construction stage are memory bounded.
5 SLOSHING FLUID CONTAINED IN LNG VESSEL TANKS

In order to provide a practical application case, the sloshing in a rectangular LNG vessel tank has been simulated. Sloshing moment amplitudes in a rectangular tank for a wide range of rolling frequencies have been investigated experimentally and numerically, see [11] or [12].

5.1 Problem description

The experimental data were measured in a tank (62 mm thickness) similar to the one shown in Figure 4, where only a lateral water impact has been considered.

Fixed particles (also refereed as dummy particles) have been used to impose the boundary condition. This type of boundary condition has a simple implementation in a massive parallel oriented code, but the consequences of this solution could be improved if more sophisticated boundary conditions are implemented.

The physical time simulated was 3 seconds (First impact time scale) and the number of particles \( N \) was around 100000. The computational time using a NVIDIA GeForce GTX 295 was less than 2 hours. This device has 480 cores, but excepting Multi-GPU implementation, only 240 cores can be used simultaneously.

To take into account the action of the engine that causes the tank movement, which
is not a pure sinusoidal signal, and include all this effects in the simulation, the moving parameters of the tank (angle, angular velocity and angular acceleration) were directly obtained from the benchmark. This methodology tries to include the initializing phase caused by engine start in the fluid simulation.

5.2 Results

In figure 5, the pressure(left) and velocity (right) fields are represented in a zoomed area where the pressure sensor measures the first wave impact. Although the velocity field is nicely smoothed, the pressure field still has the typical noise effect present in weakly compressible SPH simulations.

Looking at figure 5 two interesting effects can be observed, firstly, the distance between particles is not kept constant and density instabilities are present at the free surface, secondly the particles are unable to reach the wall boundary and an undesired gap appears between the wall and the closest particles.

In Figure 4 the complete distribution of sensors in the tank is shown. In this work only the sensor 1 has been used for the validation.

In order to improve the pressure measurement, Shepard correction [13] has been implemented to improve the consistency of the interpolation, getting at least a 0th order consistency.

During the simulation, two different parts can be distinguished, in the first one the sensor 1 records the result of a nearly hydrostatic pressure distribution, in the second part the violent impact is registered and the flow dynamics is extremely complex. Comparing the results obtained, see Figure 6, when fixed particles are taken into account in sensor pressure interpolation the hydrostatic part of the simulation has a good agreement with the experimental data. This fact contrasts with the second part where the impact pressure measurement is better represented without fixed particles in the interpolation. When no fixed particles are taken into account for the pressure interpolation, the error in the maximum pressure impact value is around 870 Pa/m (24%). It was also noticed that the maximum pressure impact simulated was delayed 0.06 seconds compared to the experimental wave impact.
6 CONCLUSIONS

A CPU-GPU solver has been developed to deal with 2D free surface flow problems requiring high computational cost. This code can be run as either a CPU code or a GPU code depending on the availability of hardware. The model has been demonstrated to be both accurate and efficient when dealing with a gravity-dominated flow problem. The code was tested in two different problems: first, the classical dam-break problem and also, the wave impact of the sloshing fluid contained in LNG vessel tanks as a practical example of particle methods. Simulations carried out for different resolutions showed a close agreement between numerical and experimental results. In addition, the numerical results were observed to converge to the experimental ones when increasing the resolution (the number of particles), both for free-surface elevations and pressures. In terms of efficiency, we have demonstrated that simulations with a large number of particles can be simulated on a personal computer equipped with a CUDA-enabled GPU card taking advantage of the performance and memory space provided by the new GPU technology. This means that research can be conducted with available cheap technology for problems that previously required high-performance computing (HPC). The speedups obtained in this work reveal the possibility to study real-life engineering problems at a reasonable computational cost. For the validation case chosen here, the GPU parallel computing can accelerate serial SPH codes by almost two orders of magnitude. Experience has shown that the speedup varies from one test to another with even greater speedup achievable than found here. The achieved performance can be compared to the large cluster machines, which are expensive and hard to maintain. Finally, for simulations requiring several million particles the immediate future for GPU computing should focus upon multi GPU implementations, since the memory requirements are still a limitation for a single GPU.

REFERENCES


THE APPLICATION OF LAGRANGIAN VORTEX METHODS TO THE
PREDICTION OF HYDRODYNAMIC DAMPING OF FLOATING
BODIES

J. MICHAEL R. GRAHAM*

* Department of Aeronautics, Imperial College,
London SW7 2AZ, UK
e-mail: m.graham@imperial.ac.uk

Key words: Hydrodynamic Damping, Vortex Shedding, Roll Motion.

Summary. Lagrangian vortex methods of simulating the vortex shedding which occurs at the bilges and sharp edges of floating bodies under oscillatory flow conditions due to incident waves and motion of the body in response are presented. Local forces are taken from discrete vortex simulations of the flow around an isolated edge representing the bilge section of the hull. Both the classical, meshless, potential flow vortex method and a vortex-in-cell viscous simulation are used. The flow around the bilge of a typical long floating hull in beam waves is treated on a sectional basis and the isolated edge results are matched to the outer three-dimensional wave potential flow provided by a standard surface panel method. The advantage of this matching procedure is that the more computationally expensive vortex flow simulation is limited to the local bilge section for which universal results may be computed whereas the large scale wave-hull interaction which extends out many hull- or wave-lengths from the body is solved by the less computationally intensive panel method. This procedure thus provides an efficient method replacing empirical vortex damping coefficients, as presently used, by a more rational method based on flow physics. Results for regular waves generating sinusoidal flows around right angle edges, edges fitted with flat plate bilge keels and rounded edges are presented and some comparisons made with measured data from laboratory wave tank tests and results of full Navier-Stokes simulations.

1 INTRODUCTION

Viscous forces usually need only be considered when predicting hydrodynamic forces on a floating body in oscillatory flow without mean velocity when the relevant Keulegan-Carpenter number, \( U_0 T / b \), is much greater than one. Here \( U_0 \) is the amplitude of relative velocity of the incident waves and/or oscillatory body motion, \( T \) the period and \( b \) a relevant length, typically the beam. Because of amplitude limits on \( U_0 \), due for example to wave breaking, viscous forces are usually much smaller than wave potential forces unless the body is ‘small’ enough not to be in the wave diffraction regime. However it is well established that for certain body motions the viscous component of the damping, although small relative to
total wave potential forces, determines the response amplitude of the body because the latter are principally inertia forces with very little contribution to damping. The best known example is the roll damping of ship or barge hulls in beam waves. Other important cases include slow drift motions in sway and surge and damping of the free surface elevation in moonpools.

Viscous damping arises from both direct boundary layer effects (skin friction and displacement) and also from the effects of flow separation on the pressure distribution. The direct boundary layer effects are normally negligible at full scale but may be important in model tests. Flow separation usually occurs in cross-flows about local regions of high curvature on the body surface such as the bilges. For sufficiently sharp edges (right angles, bilge keels) the separated flow is essentially independent of the Reynolds number and an inviscid treatment is possible, but if the edges are rounded a viscous treatment is required.

Navier-Stokes computations have been carried out for entire separated flow fields of this type including the free surface [eg. 1, 2]. A disadvantage of a full Navier-Stokes field computation including the body and the relevant extent of the free surface is the large flow domain which must be simulated. This should cover several wavelengths of the incident waves for minimum effect of domain truncation at the outer boundaries. The present method, described here, takes advantage of Greens function methods to solve the wave potential field which is the major part of the flow field for which the effects of viscosity may be neglected. These methods impose the correct outer radiation conditions for the wave field through the choice of Greens function without the need to consider any finite outer boundary. The viscous part of the calculation can then be limited to a smaller inner flow field. The flow in this region may be computed by a method, suitable for the separated and/or viscous flow, which is matched to the outer potential flow field in a similar manner to classical boundary-layer theory.

2. METHOD OF ANALYSIS

The method embeds a solution of the inner viscous flow field within the outer potential flow following a Helmholtz split of the velocity field. It is convenient to consider the case of non-steep waves:

$$H(\text{waveheight})/L(\text{wavelength}) = \varepsilon << 1,$$

so that the wave potential flow can be treated by linearised analysis.

For the present case a slender floating body is assumed with length much greater than beam $b$, assumed to be $O(L)$ so that the body is not small with respect to the wave field and therefore in the diffraction regime. The response amplitude due to the waves is $O(H)$ and it is assumed that the body has one or more edge regions of small radius of curvature, $R << b$ (eg. bilges). A (non-unique) Helmholtz split of the flow field is made by writing:

$$U(x,t) = \nabla \phi + U_r$$

(1)

The potential flow field $\phi$ is obtained from any Greens function method for the incident, diffracted and radiated fields satisfying the normal velocity boundary condition zero relative to the body surface for the incident and diffracted waves and all the degrees of freedom in
which the body responds. This outer flow drives an inner rotational flow field $U_r$ satisfying modified equations:

$$\frac{\partial U_r}{\partial t} + U_r\nabla U_r = -\frac{1}{\rho} \nabla p + \nabla^2 U_r$$

(2)

with boundary conditions on the body surface ($\mathbf{n}$ normal, $\mathbf{s}$ tangential):

$$U_r\cdot\mathbf{n} = 0 \quad \text{to satisfy zero normal velocity and}$$

$$U_r\cdot\mathbf{s} = -\frac{\partial \phi}{\partial \mathbf{s}} \quad \text{to remove the outer flow slip velocity.}$$

The inner flow field for a long body in beam waves, typically the worst roll/sway/heave case for a ship or barge hull, varies slowly ($O(\text{beam/length})$ in the lengthwise direction compared with the cross-sectional variation and may be approximated, as conventionally, by a series of locally two-dimensional sections (Figure 1).

![Figure 1. Strip theory showing 2-D hull sections.](image)

Therefore in each inner sectional flow:

$$\frac{\partial \omega}{\partial t} + U_r\nabla \omega = \nabla^2 \omega$$

(3)

where $\omega \equiv (\nabla \times U_r)_1$, the dominant component of vorticity which is in the axial direction and normal to the section.

For a sharp-edge which fixes the separation and a high Reynolds number, the viscous term in equation 3 may be neglected since the effects of skin friction and diffusion of shed vortices are small. Therefore:

$$\frac{D\omega}{Dt} \equiv \frac{\partial \omega}{\partial t} + U_r\nabla \omega = 0$$

(4)

This equation used together with the Biot-Savart law to compute inviscid oscillatory flow around a sharp right-angle edge is the classical two-dimensional discrete vortex method.
which the body responds. This outer flow drives an inner rotational flow field $U_r$ satisfying modified equations:

$$U_{rp} U_t + \nabla \cdot \mathbf{u} = 0$$

with boundary conditions on the body surface (n normal, s tangential):

$$U_r.n = 0 \quad \text{to satisfy zero normal velocity and}$$

$$U_r.s = -\frac{\partial \phi}{\partial s} \quad \text{to remove the outer flow slip velocity.}$$

The inner flow field for a long body in beam waves, typically the worst roll/sway/heave case for a ship or barge hull, varies slowly ($O(\text{beam/length})$ in the lengthwise direction compared with the cross-sectional variation and may be approximated, as conventionally, by a series of locally two-dimensional sections (Figure 1).

![Figure 1. Strip theory showing 2-D hull sections.](image)

Therefore in each inner sectional flow:

$$\omega = \nabla \times u$$

where $\omega \equiv \left(\nabla \times U_r \right)/H$, the dominant component of vorticity which is in the axial direction and normal to the section.

For a sharp-edge which fixes the separation and a high Reynolds number, the viscous term in equation 3 may be neglected since the effects of skin friction and diffusion of shed vortices are small. Therefore:

$$D\omega/Dt = \nabla \cdot (\mathbf{u} \times \omega)$$

This equation is used together with the Biot-Savart law to compute inviscid oscillatory flow around a sharp right-angle edge is the classical two-dimensional discrete vortex method (DVM) in which Lagrangian point vortex particles with unchanging circulation convect the vorticity field in the cross-section as the flow develops in time. Discrete vortices shed from the separation point are made to satisfy a Kutta-Joukowski condition at the edge to represent the separating vortex sheet convecting with the local velocity field. The evolution equations are time-stepped using a second order Runge-Kutta method. An instance of the resulting vorticity distribution (figure 2) shows how the vortex structures tend to form one counter-rotating pair per flow cycle, which convects away from the edge under its own self-induced velocity, when the driving (outer) flow field is oscillatory. The case shown is from a random sequence of waves incident on a right-angled bilge fitted with a small bilge-keel.

![Figure 2. Vortex shedding generated by oscillatory flow around an isolated 90° edge representing a bilge with small bilge-keel (DVM computation).](image)

For a given geometry, right angled edge or right-angled edge plus bilge keel a single computation for a sinusoidal outer flow or a random oscillatory velocity sequence with specified characteristic period $T$ can be used through matching to provide the force on each ship hull section. To calculate the response of the floating body the procedure first computes the potential flow and the body response amplitudes to the incident and diffracted wave potential. This is then applied as an outer boundary condition to the inner rotational flow field in the time domain to provide the viscous force contribution to be added to the wave potential forces. In the case of a sharp-edged bilge this inner flow field need only be computed once since the flow field is solely a function of the non-dimensional time $(t/T)$ and the edge angle (usually $90^\circ$). A universal force may therefore be applied through a geometric scaling relationship for any hull cross-section having the same bilge edge angle. A rounded bilge or one fitted with a bilge keel has an additional length scale (radius of curvature or length of bilge keel) which formed into a Keulegan-Carpenter number provides another dimensionless parameter. The combined force on the body is then input into the time domain matrix equation for the body dynamics (for the three transverse degrees of freedom: heave, sway and roll, in the present case). The response amplitudes are recomputed and the whole procedure iterated to convergence which is rapid (less than ten iterations at roll resonance).
3. RESULTS

Figure 3 shows the roll response amplitude operator (RAO) for a rectangular section transport barge in regular beam waves, where the vortex damping has been computed using the above isolated edge technique matched to a linearised outer wave potential panel method. This compares well with laboratory wave-flume tests\(^5\) on a 1/124 scale model. But the peak ‘potential’ RAO which neglects vortex damping is about double the measured value.

Figure 3. Roll RAO (free roll) for a rectangular section barge hull with sharp bilges in regular waves, computations: o, measured : +\(^9\).

Figure 4. Ratio of rounded edge damping force coefficient to sharp edge value. Isolated edge, present DVM computations: o, previous\(^6\) : +.
In the case of a rounded bilge viscous effects reduce the strength of the vortex shedding and hence the vortex induced damping force. It is only then possible to use the inviscid DVM approach as above if the separation point on the rounded edge is specified empirically, usually at the middle of the edge. The behaviour of the averaged vortex damping coefficient $A$ computed by this type of inviscid vortex computation is shown in Figure 4 compared with an earlier DVM computation$^{[6]}$. The effect of the radius of curvature $r$ of the bilge, expressed as the Keulegan-Carpenter number $K_r (≡ U_o T/r)$, on the coefficient $A$ is shown. The roll RAO for the same case as in Figure 3 but with small bilge rounding radius equal to 1% of the beam, figure 5, shows a 10% increase in the peak RAO due to the reduced damping.

Figure 5. Roll RAO (free roll) as for figure 3 but with 1% bilge rounding, shedding point specified.

Figure 6. (a) $t/T = 0.72$ (b) $t/T = 1.44$
Vortex shedding due to sinusoidal flow around a bilge with small rounding. (VIC, major vortices visualised: $K_r = 20$, $R_r = 100$).
A better but computationally more expensive alternative for rounded edges is to solve the viscous vorticity equation including no-slip on the body surface and separation of the boundary layers, rather than using inviscid results with specified separation. For this a vortex-in-cell (VIC) method\cite{7} on a mesh of non-uniform quadrilateral cells has been used to simulate vortex shedding driven by sinusoidal flow about a slightly rounded edge as a function of two edge parameters, Keulegan-Carpenter number $K_r$, and Reynolds number $R_r \equiv U_0 r/\nu$. Figure 6 shows the vorticity field shedding from the edge with vortex pairing developing at two time instances.

Going beyond the local edge matching method the inner region may be extended completely round the hull section and up to the mean free-surface. As the region is now bigger and lacks the universality of the infinite edge it is much more expensive to compute but a more accurate option if the hull section geometry is complex. The flow field may be simulated by the same methods as before ranging from the DVM up to use of a full Navier-Stokes field solver. An example of the latter is the spectral-element method ($Nektar$\cite{8}) providing a very accurate computation of the inner flow field. Because the waves are linearised for the outer flow a simple rigid lid normal velocity boundary condition for $U_r$ has been applied on the mean free surface. This therefore excludes free-surface interactions such as the $O(\varepsilon)$ far field waves radiated by the viscous flow field.

![Figure 7. Inner region mesh for Spectral Element Navier-Stokes computation.](image)

Figure 7 shows the mesh used to compute the inner flow field. Examples are shown of two flow fields computed\cite{9} using this mesh and a variation. In the first (Figure 8) for a hull section with bilges which have very small rounding ($r/b = 0.01$) the structures of numerous shed vortex pairs are seen to be clearly visible in the inner region after several flow cycles. It should be noted that a counter-rotating vortex pair of nearly equal strength which has been shed and stopped growing exerts very little force on the body. In the second case (Figure 9) a hull section with a comparatively large radius of curvature bilge rounding ($r/b = 0.125$) shows much weaker vortex separation and shedding.
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4. CLOSING REMARKS
A range of methods have been presented for predicting roll motion damping and response of a floating hull in waves based on simulating the separation and vortex shedding which occurs at the bilges of the hull and often dominates the damping forces. All of the methods used except the final one which uses a high order finite element analysis of the Navier-Stokes equations are based on Lagrangian vortex representations of the separated flow. Two-dimensional strip theory analysis, conventional for long ship hulls, has been used throughout for the inner region. The same two-dimensional analysis of the inner separating flow is also appropriate for more general bodies provided the shedding regions can be considered relatively straight compared with the cross-flow dimensions of these regions around the edge. This would be true, for example, of a spar buoy with a truncated vertical, circular, cylindrical geometry but not of a region near the bow or stern of a ship hull.
5. REFERENCES.
EXPERIMENTAL AND NUMERICAL ANALYSIS OF DEVELOPER FLOW IN A DEVELOPING MACHINE

MASAYUKI TANAKA*, TAKAYUKI MASUNAGA*, TAKESHI WATANABE† AND KOICHIRO SATO†

* Corporate Manufacturing Engineering Center, Toshiba Co., Ltd
33, Shinisogo-cho, Isogo-ku, Yokohama-shi, Kanagawa, JAPAN
e-mail: masayuki11.tanaka@toshiba.co.jp

† Toshiba Tec Corporation
6-78 Minami-cho, Mishima-shi, Shizuoka, JAPAN

Key words: DEM, Developer, Friction, van der Waals Force, Hamaker Constant

Abstract. Behaviors of developers flowing in a simplified developing machine was analyzed by evaluating torques of mixers in both experiments and numerical simulations in this research. In spherical and non-cohesive particles, the simulation result is in good agreement in the experimental result by adjusting the coefficient of friction. In non-spherical or cohesive particles, the simulation result can coincide with the experimental result by adjusting the coefficient of friction and Hamaker constant.

1 INTRODUCTION

In the developing machine of MFP (Multi Function Peripheral), the developer is circulated by rotating two mixers as shown in Fig.1. The developer, consisting of billions of toners and carriers ranging from 5 to 50 \( \mu \text{m} \) in diameters, is needed to be transferred stably and mixed thoroughly by rotating mixers. However, the behaviors of discrete particles are so complicated that it requires much time and labor to optimize the rotational velocity of mixers, the quantity of developers and the design of the developing machine experimentally. Therefore a numerical method which can predict the particle behaviors is needed in order to reduce the number of experiments and accelerate the product development speed. A non-Newtonian fluid simulation had been applied to simulate the developers, however, the results were not in good agreement with the granular behaviors well.

In this research, DEM (Discrete Element Method) [1] was applied to simulate the developers since granular materials could not be simulated well by a fluid simulation. However, there are some problems in DEM to simulate the developer flow. Firstly, the accuracy of DEM has not been validated sufficiently. Secondly, the way to choose the simulation
parameters has not been confirmed yet. Therefore, the objective of this research is to validate the DEM accuracy and to develop a method to determine the simulation parameters by comparing results of experiments and simulations. Experiments were conducted using a simplified developing machine to find out the relationship between the rotational velocity and the torque on the mixers. The corresponding numerical simulations were also performed, where the coefficient of friction and Hamaker constant were parameterized.

2 EXPERIMENTS

The outline of experiments is shown in this section. A conceptional image of the simplified developing machine, which was used in this research, is shown in Fig.1. In the real developing machine, the mixed toners and carriers are transferred, however, toners are so small that it is difficult to analyze the developer. Therefore the toner was neglected in this research, in other words, single kind of particles in each experiment was circulated. Three kinds of experiments were conducted, whereby 40 µm of carriers, 100 µm of Zirconia balls and 800 µm of Zirconia balls were used respectively. The properties of the carriers and the Zirconia balls are shown in Table 1. The carrier is non-spherical and on the other hand the Zirconia ball is spherical which is easier to analyze.

The torques on the mixers were measured. The rotational velocity of mixers ranged from 50 to 300 rpm. Although the densities of carriers and Zirconia balls are different, their volumes are almost the same, having 230 grams of carriers and 300 grams of Zirconia balls. The results of experiments are shown Fig.2.

In 800 µm of Zirconia balls, the torque increased as the rotational velocity increased. Reversely, the torque decreased in 40 µm of carriers. In 100 µm of Zirconia balls, the torque is not dependent on the rotational velocity. This is the intermediate property between 800 µm of Zirconia balls and 40 µm of carriers. It is supposed that the torque tends
Table 1: Properties of particles

<table>
<thead>
<tr>
<th></th>
<th>carrier</th>
<th>Zirconia</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter $\mu$m</td>
<td>40</td>
<td>100 &amp; 800</td>
</tr>
<tr>
<td>Density $kg/m^3$</td>
<td>4700</td>
<td>6090</td>
</tr>
<tr>
<td>Mass g</td>
<td>230</td>
<td>300</td>
</tr>
<tr>
<td>Shape</td>
<td>Non-Spherical</td>
<td>Spherical</td>
</tr>
</tbody>
</table>

Figure 2: Torque versus the rotation velocity in the experiments

to decrease more in the smaller particles as the rotational velocity increases. However, it still remains unknown whether the relationship between the torque and the rotational velocity is caused by the particles size itself or that the cohesive force increases as the particles gets smaller.

The magnitude of torques were similar in 800 and 100 $\mu$m of Zirconia balls. However, the torque of carriers was about twice larger than that of Zirconia balls. There are three explanations. Firstly, the coefficients of friction are different between carriers and Zirconia balls and the coefficient of friction of carriers might be greater than that of Zirconia balls. Secondly, the carrier is not spherical and the shear forces would act greater than Zirconia balls. Lastly, the carrier is so small that the cohesive force can not be neglected.

3 SIMULATIONS

Corresponding simulations were performed. The diameter of simulation particles was 800 $\mu$m. 800 $\mu$m of Zirconia balls were spherical and cohesive forces were neglected and therefore they can be simulated directly using DEM accurately. Some simulations were
conducted using different coefficients of friction, the torque was matched well with the experimental results when the coefficient of friction was 0.40 as shown in Fig.3. It is cleared that the coefficient of friction in simulation is determined uniquely using spherical and non-cohesive particles.

![Figure 3: Torque versus the rotation velocity in some frictions](image)

In the case of the particle diameter below 100 µm, too much particles exist to be simulated. Moreover, cohesive forces can not be ignored in such small particles and the phenomena come to be complicated. Sakai[2] has proposed a method to simulate the van der Waals forces of actual fine particles using larger particles in simulations. In this method, the van der Waals force between particles is represented as

\[ F = \frac{H^* L}{12h^2} n \]  

(1)

where \( L \) is the particle diameter, \( h \) the distance between particle surfaces, \( n \) normal direction. \( H^* \) represents Hamaker constant in simulations. In the Sakai’s formulation, when the diameter in a simulation is \( l \) times larger than the actual one, Hamaker constant in a simulation \( H^* \) should be

\[ H^* = l^3 H \]  

(2)

where \( H \) is Hamaker constant as the physical property. Since the actual Hamaker constant is unknown, Hamaker constant in a simulation is treated as a simulation parameter and adjusted to fit torques between experiments and simulations. Note that the difference of contact forces between particles as the size of particles is assumed to be neglected.
The simulation results using some Hamaker constants are shown in Fig. 4. When Hamaker constant is zero and neglecting the cohesive force, the torque increased as the rotational velocity increased. This result was well agreed with the one of 800 \( \mu \text{m} \) of Zirconia. When the van der Waals forces were considered, particle behaviors changed. When Hamaker constant is 2.0e-18 J, the simulation result was in good agreement with the result of 100 \( \mu \text{m} \) of Zirconia balls. When Hamaker constant is 9.0e-18 J, the simulation result was in good agreement with the result of 40 \( \mu \text{m} \) of carriers.

![Figure 4: Torque versus the rotation velocity in some Hamaker constants](image)

4 DISCUSSIONS

In Zirconia balls, the coefficient of friction could be determined using non-cohesive large particles. Therefore Hamaker constant could be determined uniquely to make simulation results agree with the experimental results. However, the coefficient of friction and Hamaker constant could not be determined uniquely since the frictional force and the cohesive force could not be separated. There is supposed to be many combinations of the two parameters.

Another problem is that the carrier is not a spherical particle. In this case, the shearing force is greater and the particle shape should be modeled somehow. The shape model and the method to determine the two parameters uniquely are future works.

5 CONCLUSIONS

Experimental and numerical analyses of developer flows using simplified developing machine were conducted. The simulated torques of carriers and Zirconia balls were in good agreement with the experiment results. Using spherical and non-cohesive large...
particles, the torque was in good agreement with the experiments and the coefficient of friction could be determined uniquely.

To consider cohesiveness and change Hamaker constant, the torque of actual fine particles can be simulated accurately. However, there are still some problems such as the particle shape and the method to determine parameters uniquely.

REFERENCES


FINITE POINTSET METHOD (FPM): OPTIMIZED MESHFREE SOLVER FOR AIRBAG DEPLOYMENT SIMULATIONS

JÖRG KUHNERT*, LARS ASCHENBRENNER† AND ALAIN TRAMEÇON#

* Fraunhofer Institut für Techno- und Wirtschaftsmathematik (ITWM)
Fraunhofer Institute for Industrial Mathematics
Fraunhofer Platz 1, 67663 Kaiserslautern, Germany
e-mail: joerg.kuhnert@itwm.fraunhofer.de, www.itwm.fraunhofer.de

† Volkswagen AG
38436 Wolfsburg, Germany
email: lars.aschenbrenner@volkswagen.de, www.volkswagen.de

# Engineering Systems International, ESI Group
99 rue des Solets, 94513 Rungis, France
email: atr@esi-group.com, www.esi-group.com

Key words: Meshfree Methods, General Finite Difference Scheme, Airbag Deployment.

Abstract. This document provides an outline of the complete numerical scheme of the Finite Pointset Method (FPM), a meshfree general Finite Difference idea to simulate gasdynamics. The method uses a specialized upwind formulation as well as specialized discrete numerical differential operators in order to gain accuracy as well as stability. The scheme is completed by a k-epsilon turbulence model in order to account for viscous effects. Industrially, FPM performs in airbag deployment modelling as a part of full crash simulations in vehicle design and development.

1 INTRODUCTION

The Finite Pointset Method (FPM) is a generalized numerical tool for simulations in fluid and continuum mechanics. It uses a generalized least squares approach for numerical approximation of derivatives on non-structured point clouds. This procedure turns out to be a generalized finite difference idea with the interesting effect that it reduces to classical finite differences, if the points would be placed in a regular grid.

The character of FPM is Lagrangian, i.e. the particles (points) of the point cloud move with fluid velocity. This turns the method into a very adaptive tool, especially regarding moving parts of the geometry and free surfaces.

In this article, we show how to develop an FPM scheme for compressible fluid flow with viscous effects as well as turbulence modelling. In fact, the differential equations have a strongly hyperbolic character, such that we need to provide a clever upwind scheme (section 2). The numerical integration of turbulences provides the main partition of the system’s viscosity and, therefore, requires particular attention (section 3). The special meshfree
(general finite difference) operators used by FPM are explained in section 4. The whole method is industrially applied for airbag deployment simulations in many vehicle manufacturing companies (section 5).

Nomenclature: throughout the paper, a tilde sign (~) in conjunction with differential operators always mean the numerical approximation by the FPM-specialized numerical differential operators.

2 NUMERICAL SCHEME FOR COMPRESSIBLE GASDYNAMICS IN LAGRANGIAN FORM

For modelling gas dynamics flows, we have to consider the laws for conservation of mass, momentum, and energy. Their representation in differential form can be written down in material derivatives (change of the values along a particle path), also known as Lagrangian formulation. FPM will make use of this because it is based on a cloud of numerical points that move with fluid velocity.

2.1 Differential equations to be considered

Let us first have a look at the differential equations of flow motion to be considered here.

General 3D Euler equations (no viscosity)

The general 3D Euler equations for inviscid gas dynamics on a Lagrangian basis are

\[
\frac{\partial}{\partial t} \rho + \rho \cdot \nabla \cdot \mathbf{v} = 0 \\
\frac{\partial}{\partial t}(\rho \mathbf{v}) + (\rho \mathbf{v}) \cdot \nabla \mathbf{v} + \nabla p = 0 \\
\frac{\partial}{\partial t}(\rho E) + (\rho E) \cdot \nabla \mathbf{v} + \nabla \cdot (p \cdot \mathbf{v}) = 0
\] (1)

The variables used are

\[
\rho = \text{density, } \rho \mathbf{v} = \text{momentum, } \rho E = \rho \int c_v dT + \frac{1}{2} \rho (\mathbf{v}^T \cdot \mathbf{v}) + k = \text{total energy,}
\]

\[
\mathbf{v} = (u \ v \ w)^T = \text{velocity vector, } p = \text{pressure, } k = \text{turbulent kinetic energy}
\]

Resulting 1D scheme in primitive form

Let us first assume that there are no turbulent effects, i.e. \( k = 0 \). Out of (1), the resulting 1D scheme is

\[
\frac{\partial}{\partial x} (\rho) + \frac{\partial}{\partial x} \left( \rho u \right) = 0
\]

\[
\frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial x} \left( \rho u^2 + p \right) = 0
\]

\[
\frac{\partial}{\partial x} (\rho E) + \frac{\partial}{\partial x} \left( \rho u E + p u \right) = 0
\] (2)

The set of differential equations (2) is in conservative form. For analytical reasons, it will be more useful in the primitive form. Hence, with the help of the thermodynamic identity
\[ \frac{d}{dt} p = \left. \frac{\partial p}{\partial T} \right|_T \left( \frac{\partial T}{\partial T} \right) + \left. \frac{\partial p}{\partial p} \right|_T \left( \frac{\partial p}{\partial T} \right) \]

and the definition of the sound speed by

\[ c^2 = \left. \frac{\partial p}{\partial T} \right|_T + \frac{p}{c^2} \left. \frac{\partial p}{\partial p} \right|_T, \]

we derive the primitive form of (2) as to be

\[ \frac{d}{dt} \rho + \frac{p}{c^2} \frac{\partial \rho}{\partial x} = 0 \]

\[ \frac{d}{dt} u + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0 \]

\[ \frac{d}{dt} p + \rho c^2 \frac{\partial u}{\partial x} = 0 \]

### 2.2 Derivation of a scheme 1D scheme by characteristic analysis

The system (3) is perfect for numerical analysis. We would like to establish a stable scheme for this system, well knowing that it is of hyperbolic character. If we are applying a centralized FPM scheme (i.e. using centralized approximations for the occurring derivatives \( \frac{\partial u}{\partial x} \) and \( \frac{\partial p}{\partial x} \)), then we will encounter unstable behaviour of the numerical solution. We suggest therefore a local numerical viscosity in order to stabilize the scheme. First, we need to decouple the system of equations (3) into separate, characteristic differential equations. In compact form, the equations (3) can be written down as

\[ \frac{dV}{dt} + M \cdot \frac{\partial V}{\partial x} = 0 \]

The matrix \( M \) can be decomposed into its eigenvectors \( L \cdot M = \Lambda \cdot L \), and we explicitly have

\[ V = \begin{pmatrix} \rho \\ u \\ p \end{pmatrix}, \quad M = \begin{pmatrix} 0 & \rho & 0 \\ 0 & 0 & 1/\rho \\ 0 & \rho c^2 & 0 \end{pmatrix}, \quad \Lambda = \begin{pmatrix} 0 & c \\ c & -c \\ 0 & -\rho c \end{pmatrix}, \quad L = \begin{pmatrix} -c^2 & 0 & 1 \\ 0 & \rho c & 1 \\ 0 & 0 & -\rho c \end{pmatrix} \]

Thus, (4) appears as

\[ L \cdot \frac{dV}{dt} + \Lambda \cdot L \cdot \frac{\partial V}{\partial x} = 0, \]

and the resulting scheme in expanded form can be written as

\[ -c^2 \frac{d}{dt} \rho + \frac{d}{dt} p = 0 \]

\[ \frac{d}{dt} \left( \rho u + p \right) + c \frac{\partial}{\partial x} \left( \rho u + p \right) = u \left( \frac{d}{dt} \rho c + c \frac{\partial}{\partial x} \rho c \right) \]

\[ \frac{d}{dt} \left( -\rho u + p \right) - c \frac{\partial}{\partial x} \left( -\rho u + p \right) = -u \left( \frac{d}{dt} \rho c - c \frac{\partial}{\partial x} \rho c \right) \]
The scheme (7) consists of several, uncoupled scalar differential equations, each of which represent a separate transport task of the form

$$\frac{d}{dt} \phi \pm c \cdot \frac{\partial \phi}{\partial x} = 0$$  \hspace{1cm} (8)

for the dedicated pieces of information $\phi = (\rho cu+p)$, $\phi = (-\rho cu+p)$ as well as $\phi = \rho c$, also referred to as the characteristic items. The term $\pm c$ is the corresponding, characteristic speed of transport. It is not surprising, that its absolute value for each of the single characteristic items turns out to be the sound speed.

**Upwind scheme leading to local viscosity terms**

A very simple and stable explicit numerical scheme for (8) is

$$\phi_{n+1}^i = \phi_n^i \left( x_i \right) = \phi_n^i \left( x_i \pm c \cdot \Delta t \right), \hspace{1cm} (9)$$

with the time step size $\Delta t$. "i" is the particle index and “n”, “n+1” represent the discrete time levels. The value of the term $\phi_n^i \left( x_i - c \cdot \Delta t \right)$ cannot be provided immediately, either a precise numerical, least squares-like approximation of the quantity $\phi$ at the location $(x_i \pm c \cdot \Delta t)$ can be provided such that the scheme turns out to be $\phi_{n+1}^i = \tilde{\phi}^i \left( x_i \pm c \cdot \Delta t \right)$, or by a Taylor-series expansion we find $\phi_n^i \left( x_i - c \cdot \Delta t \right) = \phi_n^i \left( x_i \right) - c \cdot \Delta t \left[ \frac{\partial \phi}{\partial x} \right] + \frac{(c \cdot \Delta t)^2}{2} \left[ \frac{\partial^2 \phi}{\partial x^2} \right] + \text{HOT}$. By using again the least squares approximations for the derivatives and neglecting the higher order terms (HOT), the numerical solution turns out to be

$$\phi_{n+1}^i = \phi_n^i \pm c \cdot \Delta t \left[ \frac{\partial \phi}{\partial x} \right] \pm \frac{(c \cdot \Delta t)^2}{2} \left[ \frac{\partial^2 \phi}{\partial x^2} \right]$$ \hspace{1cm} (10)

In other words, scheme (10) is a first order approximation of a model equation, which enhances (8) by a diffusion term:

$$\frac{d}{dt} \phi \pm c \cdot \frac{\partial \phi}{\partial x} = \frac{\partial \eta}{\partial x} \left( \phi \cdot \frac{\partial \phi}{\partial x} \right)$$ \hspace{1cm} (11)

The right hand side can be considered as the numerical viscosity, the simplest choice is, due to (10), given by $\eta = \frac{c^2 \cdot \Delta t}{2}$. However, $\eta$ accounts also for the higher order terms, and thus, in a more general sense, we establish a local quantification of $\eta$ by first numerically solving (8) without viscosity and assigning local values of $\eta$ based on the local overshoots or instabilities. The final numerical solution for one time step is then produced by integration of equation (11).

**Stabilized 1D scheme**

Numerical stabilization of the scheme (7) naturally follows from (11) by enhancing the transport terms by the numerical viscosity terms:
\[-c^2 \frac{\partial}{\partial t} \rho + \frac{\partial}{\partial t} p = 0\]

\[
\frac{\partial}{\partial t} (p + \rho u) + c \cdot (p + \rho u) = \left( \frac{\partial}{\partial t} (\rho c) + c \cdot (\rho c)_x \right) + \left( \eta^+ (p + \rho cu)_x \right)_x - u \left( \mu^+ (\rho c)_x \right)_x
\]  \hspace{1cm} (12)

\[
\frac{\partial}{\partial t} (p - \rho u) - c \cdot (p - \rho u) = -u \left( \frac{\partial}{\partial t} (\rho c) - c \cdot (\rho c)_x \right) + \left( \eta^- (p - \rho cu)_x \right)_x + u \left( \mu^- (\rho c)_x \right)_x
\]

with artificial numerical viscosity terms \( \eta^+ , \mu^+ , \eta^- , \) and \( \mu^- , \) the size of which can be determined by the locally given state. The sub-indices \( u_x \) signify, of course, least squares approximation of the derivative with respect to \( x \). Equation (12) can analytically be solved for the time change rates of density, velocity, and pressure, which results in

\[
\frac{\partial}{\partial t} \rho + \rho \cdot u_x = \frac{1}{c^2} \left( \eta p_x \right)_x
\]

\[
\frac{\partial}{\partial t} u + \frac{1}{\rho} p_x = (\eta u)_x
\]

\[
\frac{\partial}{\partial t} p + \rho c^2 \cdot u_x = (\eta p)_x
\]

where we assumed (just for simplicity!) \( \eta^+ = \mu^+ \) and \( \eta^- = \mu^- \), and even \( \eta = \eta^- + \eta^+ \). We suggest a definition of numerical velocity and pressure functions given by

\[
\bar{u} = u - \eta \cdot \frac{1}{\rho c^2} p_x
\]

\[
\bar{p} = p - \eta \cdot \rho u_x
\]

With this definition and equation (13), we find the modified, but stable, numerical system to be time-integrated

\[
\frac{\partial}{\partial t} \rho + \rho \cdot \bar{u}_x = 0
\]

\[
\frac{\partial}{\partial t} u + \frac{1}{\rho} \bar{p}_x = 0
\]

\[
\frac{\partial}{\partial t} p + \rho c^2 \cdot \bar{u}_x = 0
\]

Coming back to the conservative formulation, the above system can be represented as

\[
\frac{\partial}{\partial t} \rho = -\rho \cdot \bar{u}_x
\]

\[
\frac{\partial}{\partial t} (\rho u) = -(\rho u) \cdot \bar{u}_x - \bar{p}_x
\]

\[
\frac{\partial}{\partial t} (\rho E) = -(\rho E) \cdot \bar{u}_x - (\bar{p} \cdot \bar{u})_x
\]

2.3 Projection of the 1D scheme to the 3D case

In the same fashion as above, we find a system of equations in 3D, which is similar to the equations (16).
\[
\begin{align*}
\frac{d}{dt} \rho &= -\rho \cdot \nabla^T \mathbf{v} \\
\frac{d}{dt} (\rho \mathbf{v}) &= -((\rho \mathbf{v}) \cdot \nabla^T \mathbf{v} - \nabla^T \mathbf{p}) \\
\frac{d}{dt} (\rho E) &= -((\rho E) \cdot \nabla^T \mathbf{v} - \nabla^T (\mathbf{p} \cdot \mathbf{v}))
\end{align*}
\] (17)

The symbol \( \nabla^* \) signifies the FPM-specialized moving-least-squares (MLS) gradient operator, see also section 4. Similarly, \( \Delta^* \) for example represents the FPM-MLS approximation of the Laplace operator, which will be used later on. The numerical pressure and velocity expressions are

\[
\begin{align*}
\mathbf{v} &= (\bar{u} \quad \bar{v} \quad \bar{w})^T = \mathbf{v} - \eta_p \nabla^T \mathbf{p} \\
\mathbf{p} &= p - \eta_v \nabla^T \mathbf{v}
\end{align*}
\] (18)

By virtue of equation (14) we define

\[
\begin{align*}
\eta_p &= \eta_{num} \cdot \left( \frac{1}{\rho c^2} \right) \\
\eta_v &= \eta_{num} \cdot \rho
\end{align*}
\] (19)

We will later see, that \( \eta_{num} \) plays an important role as numerical stabilization quantity. For example, \( \eta_v \) has nearly the same character as a physical viscosity. For the present chapter, let us assume that we know the values of \( \eta_{num} \) at any location.

### 2.4 Adding viscosity to the numerical scheme

In order to treat viscous effects, that come into play for example by the consideration of turbulent motion, scheme (17) has to be enhanced by the viscous stress tensor

\[
\begin{align*}
\frac{d}{dt} \rho &= -\rho \cdot \nabla^T \mathbf{v} \\
\frac{d}{dt} (\rho \mathbf{v}) &= -((\rho \mathbf{v}) \cdot \nabla^T \mathbf{v} - \nabla^T \mathbf{p} + (\nabla^T \mathbf{S})^T) \\
\frac{d}{dt} (\rho E) &= -((\rho E) \cdot \nabla^T \mathbf{v} - \nabla^T (\mathbf{p} \cdot \mathbf{v}) + \nabla^T (\mathbf{S} \cdot \mathbf{v}))
\end{align*}
\] (20)

The viscous stress tensor in fact is a numerical model of the classical stress tensor of the form

\[
\mathbf{S} = \overline{\eta} \left( \nabla^T \mathbf{v} + (\nabla^T \mathbf{v})^T - \frac{2}{3} (\nabla^T \mathbf{v}) \cdot \mathbf{I} \right)
\] (21)

With the definition of the effective numerical viscosity, given by \( \overline{\eta} = \eta_{visc} + \eta_{turb} \). In the same fashion, the laminar viscous and turbulent partitions of the stress tensor can be defined as

\[
\begin{align*}
\mathbf{S}_{turb} &= \eta_{turb} \left( \nabla^T \mathbf{v} + (\nabla^T \mathbf{v})^T - \frac{2}{3} (\nabla^T \mathbf{v}) \cdot \mathbf{I} \right) \\
\mathbf{S}_{visc} &= \eta_{visc} \left( \nabla^T \mathbf{v} + (\nabla^T \mathbf{v})^T - \frac{2}{3} (\nabla^T \mathbf{v}) \cdot \mathbf{I} \right)
\end{align*}
\] (22)

which will be needed later on.
3 NUMERICAL INTEGRATION OF TURBULENCE

We will model the k-epsilon turbulence idea within the FPM framework.

3.1 Differential equations of the k-epsilon model

For the purpose of this paper, we will concentrate on the k-epsilon-turbulence formulation. The model equations are

\[
\frac{d}{dt}(\rho k) = \nabla^T \left( \left( \frac{\eta_{visc}}{\sigma_k} \right) \nabla k \right) - \rho \varepsilon + P_k + P_b \\
\frac{d}{dt}(\rho \varepsilon) = \nabla^T \left( \left( \frac{\eta_{visc} + \eta_{turb}}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) - C_{2e} \rho \frac{\varepsilon^2}{k} + C_{1e} \frac{\varepsilon}{k} (P_k + P_b)
\]

Here, \( P_k \) means the turbulent production rate, and it is determined by

\[
P_k = \nabla^T \left( S_{turb} \cdot \mathbf{v} \right) - \left( \nabla^T S_{turb} \right) \cdot \mathbf{v} = \eta_{turb} \cdot \| \mathbf{D} \|^2_{\alpha_f}
\]

A similar expression, \( P_b \), is dedicated to turbulent buoyancy effects, which will be neglected for this paper. The turbulent viscosity is a function of the turbulent quantities \( k \) and \( \varepsilon \), represented by \( \eta_{turb} = \rho \cdot C_\eta \cdot \frac{k^2}{\varepsilon} \). The given model constants are \( \sigma_k, \sigma_\varepsilon, C_{2e}, C_{1e}, C_\eta \), and finally,

\[
\| \mathbf{D} \|^2_{\alpha_f} = \left( v_x + u_y \right)^2 + \left( w_x + u_z \right)^2 + \left( v_x + w_y \right)^2 + 2 \left( u_x - v_x \right)^2 + 2 \left( v_y - w_y \right)^2 + 2 \left( w_z - u_z \right)^2
\]

provides, in fact, the Mises-norm of the symmetric part of the velocity gradient, which ensures that the turbulent production rate be always positive.

3.2 Numerical evolution scheme and time integration of the k-epsilon model

The numerical evolution scheme

\[
\frac{d}{dt}(\rho k) = \bar{\nabla}^T \left( \left( \frac{\eta_{turb}}{\sigma_k} \right) \bar{\nabla} k \right) - \rho \varepsilon + P_k \\
\frac{d}{dt}(\rho \varepsilon) = \bar{\nabla}^T \left( \left( \frac{\eta_{turb}}{\sigma_\varepsilon} \right) \bar{\nabla} \varepsilon \right) - C_{2e} \rho \frac{\varepsilon^2}{k} + C_{1e} \frac{\varepsilon}{k} P_k
\]

just arises by replacing the spatial derivatives in (23) by its FPM-MLS operators. For better numerical analysis, we can rewrite this scheme by replacing \( P_k \) by its formal expression (24)

\[
\frac{d}{dt}(k) = \frac{1}{\rho} \left( \bar{\Delta}_k k \right) - \varepsilon + C_\eta \frac{k^2}{\varepsilon} \| \mathbf{D} \|^2_{\alpha_f} \\
\frac{d}{dt}(\varepsilon) = \frac{1}{\rho} \left( \bar{\Delta}_\varepsilon \varepsilon \right) - C_{2e} \frac{\varepsilon^3}{k} + C_{1e} C_\eta \cdot k \cdot \| \mathbf{D} \|^2_{\alpha_f}
\]
From system (26), we derive a singularity formulation, which is either

$$\frac{d}{dt} \left( \frac{k}{\varepsilon} \right) = (C_{2e} - 1) + C_\eta \left( 1 - C_{1e} \right) \| \mathbf{D} \|_{kr}^2 \cdot \left( \frac{k}{\varepsilon} \right)^2 + \frac{1}{\rho} \left( \tilde{\Lambda}_{k} \frac{k}{\varepsilon} \right)$$  \hspace{1cm} (27)

or

$$\frac{d}{dt} \left( \frac{\varepsilon}{k} \right) = (1 - C_{2e}) \cdot \left( \frac{\varepsilon}{k} \right)^2 + C_\eta (C_{1e} - 1) \| \mathbf{D} \|_{kr}^2 + \frac{1}{\rho} \left( \tilde{\Lambda}_{\varepsilon} \frac{\varepsilon}{k} \right)$$  \hspace{1cm} (28)

If not both values $k$ and $\varepsilon$ are zero, we can provide numerical mean values

$$k \left[ k_{\text{mean}} \right] = \frac{1}{\Delta t} \int_0^{\Delta t} k \left[ \frac{\varepsilon}{k} \right] dt \quad \text{and} \quad \varepsilon \left[ k_{\text{mean}} \right] = \frac{1}{\Delta t} \int_0^{\Delta t} \frac{\varepsilon}{k} \left[ k \right] dt \hspace{1cm} (29)$$

It remains to state a possibly precise numerical time integration method of the scheme (26) where we avoid singularities by using the mean values (29). Thus, the numerical evolution scheme can be written as

$$\frac{d(k)}{dt} = \frac{1}{\rho} \left( \tilde{\Lambda}_k k \right) - \left( \varepsilon \left[ k_{\text{mean}} \right] \right) \cdot k + C_\eta \left( \frac{k}{\varepsilon \left[ k_{\text{mean}} \right]} \right) k \| \mathbf{D} \|_{kr}^2$$  \hspace{1cm} (30)

$$\frac{d(\varepsilon)}{dt} = \frac{1}{\rho} \left( \tilde{\Lambda}_\varepsilon \varepsilon \right) - C_{2e} \cdot \left( \frac{\varepsilon}{k_{\text{mean}}} \right) \cdot \varepsilon + C_{1e} C_\eta \left( \frac{k}{\varepsilon \left[ k_{\text{mean}} \right]} \right) \cdot \varepsilon \| \mathbf{D} \|_{kr}^2$$

for which we can now apply a numerical integration that guarantees the positivity of the terms $k$ and $\varepsilon$. It is based on semi-implicit first order time stepping, given by

$$\frac{k^{n+1} - k^n}{\Delta t} = \frac{1}{\rho} \left( \tilde{\Lambda}_k k^n \right) - \left( \varepsilon \left[ k_{\text{mean}} \right] \right) \cdot k^{n+1} + C_\eta \left( \frac{k}{\varepsilon \left[ k_{\text{mean}} \right]} \right) \| \mathbf{D} \|_{kr}^2 \cdot k^n$$  \hspace{1cm} (31)

$$\frac{\varepsilon^{n+1} - \varepsilon^n}{\Delta t} = \frac{1}{\rho} \left( \tilde{\Lambda}_\varepsilon \varepsilon^n \right) - C_{2e} \cdot \left( \frac{\varepsilon}{k_{\text{mean}}} \right) \cdot \varepsilon^{n+1} + C_{1e} C_\eta \left( \frac{k}{\varepsilon \left[ k_{\text{mean}} \right]} \right) \| \mathbf{D} \|_{kr}^2 \cdot \varepsilon^n$$

### 3.3 Analytical evaluation of the mean values of the singular terms

The singular terms $\frac{k}{\varepsilon \left[ k_{\text{mean}} \right]} = \frac{1}{\Delta t} \int_0^{\Delta t} k \left[ \frac{\varepsilon}{k} \right] dt$ and $\frac{\varepsilon}{k \left[ \varepsilon_{\text{mean}} \right]} = \frac{1}{\Delta t} \int_0^{\Delta t} \frac{\varepsilon}{k} \left[ k \right] dt$ need to be evaluated analytically in order to provide acceptable values for integration scheme (31). If we assume negligibility of the diffusion term $\frac{1}{\rho} \left( \tilde{\Lambda}_\eta \left( \frac{\varepsilon}{k} \right) \right)$ in equation (27), it reduces to

$$\frac{d}{dt} \left( \frac{k}{\varepsilon} \right) = (C_{2e} - 1) + C_\eta \left( 1 - C_{1e} \right) \| \mathbf{D} \|_{kr}^2 \cdot \left( \frac{k}{\varepsilon} \right)^2$$

and more simple

$$\frac{d}{dt} x = A - B \cdot x^2$$  \hspace{1cm} (32)
Here, \( x = \frac{\varepsilon}{k} \), \( A = \left( C_{2e} - 1 \right) \), and \( B = C_\eta \left( C_{1e} - 1 \right) \| D \|_M^2 \). The analytical solution to (32) is
\[
x = \sqrt{A/B} \tanh \left( \sqrt{AB} \left( t - t_0 \right) + \text{arc tanh} \left( \sqrt{B/A} x_0 \right) \right)
\] (33)
as well as
\[
x = \sqrt{A/B} \coth \left( \sqrt{AB} \left( t - t_0 \right) + \text{arc coth} \left( \sqrt{B/A} x_0 \right) \right)
\] (34)

The arctanh is defined between -1 and 1, the arccoth complementary. Hence, the choice of the solution (33) or (34) depends on \( x_0 > \sqrt{A/B} \) or \( x_0 < \sqrt{A/B} \).

### 3.4 Boundary conditions for solid walls

The solid wall particles in FPM can be treated like interior particles, with one exception: the wall particles are assumed to be shifted to the interior of the flow domain by a small value \( \alpha \cdot h \). Thus, in the model (30), the term \( \frac{1}{\rho} \left( \hat{\Delta}_\eta k \right) \) need to have an additional contribution, i.e. the contribution that comes from the fact that the velocity drops to zero exactly at the wall. In this sense, we obtain the enhanced model by
\[
\frac{d(k)}{dt} = \frac{1}{\rho} \left( \hat{\Delta}_\eta k \right) - \left( \frac{\varepsilon}{k_{\text{mean}}} \right) \cdot k + C_\eta \left( \frac{k}{\epsilon_{\text{mean}}} \right) \mathcal{D} \|_{\text{m}}^2 + \hat{n} \cdot \left( \frac{\partial k}{\partial n} - \frac{k}{\alpha \cdot h} \right) \cdot \frac{1}{\frac{1}{2} \left( \alpha \cdot h + \frac{1}{2} h \right)}
\]
\[
\frac{d(\varepsilon)}{dt} = \frac{1}{\rho} \left( \hat{\Delta}_\varepsilon \varepsilon \right) - C_{2e} \cdot \left( \frac{\varepsilon}{\varepsilon_{\text{mean}}} \right) \cdot \varepsilon + C_{1e} C_\eta \left( \frac{k}{\epsilon_{\text{mean}}} \right) \cdot \varepsilon \cdot \mathcal{D} \|_{\text{m}}^2 + \hat{n} \cdot \left( \frac{\partial \varepsilon}{\partial n} - \frac{\varepsilon}{\alpha \cdot h} \right) \cdot \frac{1}{\frac{1}{2} \left( \alpha \cdot h + \frac{1}{2} h \right)}
\]

### 4 MEHSFREE DIFFERENTIAL OPERATORS

#### 4.1 Definition of Differential operators

Let us suppose there is a pointcloud being sufficiently dense. The positions of the particles are given by \( x_i = \left( x_i, y_i, z_i \right)^T \), \( i = 1...N \), and \( N \) is the number of particles. Suppose furthermore that some function \( f \) is given only at the discrete particle locations, i.e. \( f_i \equiv f \left( x_i \right) \). The vector of discrete function values is given by \( f \equiv \left( f_1, f_2, ..., f_N \right)^T \). We call the numerical differential operators in FPM those vectors which provide an approximation of some derivative in the sense
\[
\partial^*_{\text{numerical}} f \left( x_i \right) = \hat{\partial}^* f \left( x_i \right) = \hat{\partial}^* f_i = \sum_{j=1}^N c^j_i \cdot f_j = \left( c_i \right)^T \cdot f
\] (35)

The star (*) in the equation above is a placeholder for all the numerous differential operators needed by FPM. In that aspect, \( c^0_i \) would be the numerical operator for function approximation, \( c_1^0 \), \( c_2^0 \), \( c_3^0 \) the respective operators for the x, y, and z derivatives, and \( c_4^0 \) the one for approximation of the Laplacian. Just to name the most often appearing ones. Our goal
is to develop operators which are, as shown in (35), independent on the underlying function values. Having operators which work generally for all given functions will save a lot of computation time. We also introduce a weight function which switches on the particular neighbours close to some particle $i$.

$$W_{ij} = w(r(x_i, x_j)) = w(r_{ij}) = \left\| x_i - x_j \right\| \left(\frac{1}{2}h(x_i) + h(x_j)\right)$$  \hspace{1cm} (36)

The function $h(x_i)$ is referred to as smoothing length, turning out to be the maximum interaction radius between two particles. It actually rules the local density of the particles, i.e. the mean distance between particles. We try to provide a weight function which becomes zero if $r = 1$ and one if $r = 0$ and which is n-times continuously differentiable. For example

$$w(r) = \begin{cases} (1-r^2)^{\gamma}, & \text{if } r < 1 \\ 0, & \text{otherwise} \end{cases} \hspace{1cm} (37)$$

We can write the discrete weight values on the diagonal of the so called weight matrix

$$W_i = \begin{pmatrix} w_{i1} & 0 \\ & w_{i2} \\ & \vdots \\ 0 & w_{iN} \end{pmatrix}$$  \hspace{1cm} (38)

having the discrete weights on its diagonal and zeros otherwise.

4.2 General least squares procedure for operators

We are searching for the operator $c_i$ fulfilling the least squares criterion

$$\frac{1}{2}\left\| W_i^{-1} \cdot c_i \right\|^2 = \frac{1}{2}c_i^T \cdot W_i^{-1} \cdot W_i \cdot c_i = \frac{1}{2}c_i^T \cdot W_i^{-2} \cdot c_i = \min$$  \hspace{1cm} (39)

under the consistency conditions

$$K_i^T \cdot c_i = b$$  \hspace{1cm} (40)

The matrix $K_i$ represents test functions (given as discrete values at the particles) for which the numerical operator are forced to give a distinct value. As for example, the numerical operator for the x-derivative $c_i^x$ shall deliver zero if operating on a constant function $k_i^0 = (1, 1, \ldots, 1)$ or a quadratic function $k_i^2 = \left(x_i - x_j\right)^2, \left(x_2 - x_j\right)^2, \ldots, \left(x_N - x_j\right)^2$, but it shall deliver one if operating on the linear function $k_i^1 = \left(x_1 - x_i, x_2 - x_i, \ldots, x_N - x_i\right)$. In other words, we have the conditions (among others!)

$$\left(k_i^0\right)^T \cdot c_i^x = 0, \hspace{1cm} \left(k_i^1\right)^T \cdot c_i^x = 1, \hspace{1cm} \left(k_i^2\right)^T \cdot c_i^x = 0$$  \hspace{1cm} (41)

In general, the matrix $K$ contains $M$ discretely given test functions, which do not only contain the geometric monomials, but can be enhanced by stability conditions as well. The right hand side vector $b$ consequently contains the corresponding values to be delivered by
the operator if applied to the test functions. The minimization problem (39) together with the constraints (40) can be solved using Lagrange multipliers.

5 APPLICATIONS TO AIRBAG DEPLOYMENT

5.1 Coupling of FPM into PAM-Crash Software

FPM is linked into the crash analysis software PAM-Crash, provided by ESI Group, France. Here, FPM takes over the simulation of the gasdynamics inside of airbags, a main constructive feature in car design in order to protect drivers and passengers in case of a crash accident.

The coupling between the two codes is strong. In each simulation time step, there is a synchronization and information exchange. During one time step, FPM produces a pressure solution of the gas along the airbag’s fabrics, which is communicated to the PAM-Crash software. With this new pressure values, PAM-Crash is able to complete one time step and provide to FPM updated values of the membrane dynamics, such as position as well as velocities of the membrane’s node points. This cycle now is repeated during the whole simulation, which means that also the time step sizes of both codes have to be synchronized.
5.2 Experimental results vs. numerical simulation

The coupled method is very well validated by experiments. One typical setup is the testing of flat bags, because here any unknown factors of the folding and wrapping of airbag are excluded. In the experiment, the deploying airbag pushes away a pendulum of a certain length and mass. Experimentally, the acceleration of the pendulum is measured and later on compared to the numerical results.

5.3 Calibration of the turbulence model

The turbulence model, especially the factor $\alpha$ of section 3.4, is calibrated by experiments. They are conducted in order to correlate the pressure drop, i.e. viscous turbulent force load, inside of a tube with the according mass flux. The measurements contain the pressure difference of the beginning and end of the tube as well as localized measurements of the wall stresses. Both items can be used in order to calibrate the turbulence model, such that it at least provides the same results for these simple applications. Of course, for the experiments, the wall material of the tube is covered with airbag fabrics, such that the correct roughness of the boundaries is set into place.
INFLUENCE OF IMPACT VELOCITY ON THE FRAGMENT FORMATION OF CONCRETE SPECIMENS

DIPL.-ING. STEVE WERNER*; PROF. DR.-ING. KARL-CHRISTIAN THIENEL*

*Institut für Werkstoffe des Bauwesens (IWB)
Universität der Bundeswehr München
Werner-Heisenberg-Weg 39, 85579 Neubiberg, Deutschland
e-mail: steve.werner@unibw.de, internet: http://www.unibw.de/bauv3

Key words: Impact velocity, Fragment analyzing, Fracture surface determination

Abstract. In recent years some studies presented fragmentation models to describe the impact of projectiles [e. g.: 1, 2]. This paper shows results of high velocity impact of gun projectiles on concrete specimens. Three different muzzle velocities were tested on a standard concrete with special attention on the surface area generated. The penetration of the projectiles resulted in two craters (one on the front and one on the rear side of the specimens) and the formation of a huge number of particles of various shapes and sizes. The crater surfaces were analyzed with the 3-dimensional laser-scanner DAVID 3D which utilizes triangulation. The detailed principle is described in [3]. Parameters to describe the particles were determined with a CPA (camera particle analyzer). The used Haver CPA 2-1 is based on digital image processing with a high-resolution digital line scan camera. The following information were obtained: the shape-parameter sphericity, the particle-size-parameters (Feret-diameter, length, volume distribution) and the numbers of particles. A triaxial ellipsoid model was developed to determine the surface of the particles which takes a particle-shape-parameter into account. The main advantage of the ellipsoid model compared to the normally used sphere model is the consideration of the volume determined. The ellipsoid model provides a better picture of the real particle surfaces. Besides these sample related parameters the speed of the projectile was measured before and after penetrating the concrete specimens. As a result both kinetic energies could be calculated. Their difference corresponds to sum of the energy necessary to generate the fracture particles and their kinetic energy following the impact. In the course of this study a correlation was established between the energy difference (fracture energy + kinetic energy) and the fracture surface area generated. An increasing energy difference led to an increasing fracture surface area and higher number of particles as well. These results of the study can be utilized for designing protective concrete structures.

1 INTRODUCTION

In recent years several studies dealt with the fragmentation of different materials like steel and ceramic due to projectile impact [2, 4, 5]. If a specimen is perforated by a projectile, energy is absorbed by the specimen respectively by creating fragments of different shape and size. These fragments form fragment clouds at the front and rear side of the specimen. An overview of a few studies, which investigated the formation and propagation of fragment clouds behind thin bumpers, can be found in [2]. These studies led to models describing the
fragment clouds and the dissipated energy, but most of them dealt with metallic materials only.

The knowledge about concrete is insufficient with respect to the formation of fragment clouds. Because of the complex effects observed in impact tests on concrete the evaluation of the results is often simplified; e.g. the damage of the concrete specimen is classified simply in perforated or non perforated [6]. Other studies are more focused on the penetration depth to measure local damage. More information can be found in [7]. Nevertheless these simplified descriptions were subsequently used to determine all kinds of influences, e.g. water/cement - ratio [7, 8, 9]. The fragments were never considered.

Thus, one of the aims of this study is to analyze concrete fragments resulting from an impact perforation. A camera particle analyzer (CPA) was used for this purpose. This technique is commonly applied to sand, coal, glass, food etc. [e. g. 10, 11, 12]. Once the distribution and the shape of the fragments are known, the damage of the specimens can be described as a function of the newly created surface area. Additionally, the crater surface left in the specimens must be measured, too. This was done using a 3D laser-scanner.

Due to projectile impact a part of the kinetic energy of the projectile is converted into fracture energy creating fragments. Dinovitzer [1] divided the energy into “target plug fracture energy, projectile impact kinetic energy, target debris kinetic energy, residual penetrator kinetic energy and deformation and heat energy loss”. Schäfer [2] combined the thermally and mechanically dissipated energy and called them “dissipated” energy. In this paper the energy is only divided into the kinetic energy of the projectile and the energy difference ΔE which includes the fragment energy and kinetic energy of the fragments. The main focus was the correlation between the energy difference and the muzzle velocities of the projectiles.

2 EXPERIMENTAL INVESTIGATION

2.1 Concrete mixture and properties

A normal strength concrete mix was chosen to compare the impact effect of munition with different muzzle velocities on specimens. Details of the mix design of the concrete are given in Table 1.

<table>
<thead>
<tr>
<th>w / c [-]</th>
<th>Water [kg/m³]</th>
<th>Cement [kg/m³]</th>
<th>Sand 0 / 4 [kg/m³]</th>
<th>Gravel 4 / 8 [kg/m³]</th>
<th>Gravel 8 / 16 [kg/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6</td>
<td>185</td>
<td>310</td>
<td>847</td>
<td>364</td>
<td>680</td>
</tr>
</tbody>
</table>

The binder was a German CEM I Portland cement with a minimum strength of 42.5 N/mm² at an age of 28 days. The ratio between water and cement was 0.60. Aggregate was a limestone from a local quarry with a maximum grain size of 16 mm. For each velocity tested ten specimens were cast. The specimens were demoulded after one day and subsequently stored in lime-saturated water for 27 days until testing.
The mechanical properties were measured at 28 days. Compressive strength and Young’s modulus were determined in each case on three cylindrical specimens \((d / h = 150 / 300 \text{ mm})\) according to [13]. Three beams \((l / w / h = 100 / 100 / 500 \text{ mm})\) were used in each case to determine the bending tension strength according to [13]. The mean values of all specimens and their coefficients of variation are presented in Table 2.

**Table 2**: Mechanical properties (in parentheses: coefficient of variation)

<table>
<thead>
<tr>
<th>(\rho) [kg / dm(^3)]</th>
<th>(f_c) [MPa]</th>
<th>E [GPa]</th>
<th>(f_{ft}) [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.475 (0.002)</td>
<td>48.42 (0.016)</td>
<td>32.1 (0.011)</td>
<td>6.81 (0.037)</td>
</tr>
</tbody>
</table>

**2.2 Impact investigation**

The concrete specimens had a quadratic size of 30 x 30 cm\(^2\) and a thickness of 5 cm only. Thus, edge effects could be minimized and a perforation of the specimens due to the projectile impact was ensured. The munitions were jacketed projectiles with a hard core of tungsten carbide. Each projectile has a length of 51 mm and a diameter of 7.62 mm with a weight of 9.5 g. These projectiles are used as special munitions of the German army for the rifle HK G3.

The tests were conducted in the ballistic laboratory at the Universität der Bundeswehr München, where different ballistic test conditions could be examined. In this study the tests were carried out with a measuring weapon system (MWS) of Mauser. One advantage of this MWS is the ability to vary the muzzle velocity. The specimens were installed in a steel frame inside a backstop \((L / W / H = 2.0 / 0.7 / 0.7 \text{ m})\) of 8 mm thick steel. The distance between the MWS and the backstop was 13 m. To determine the speed of the projectiles two photoelectric barriers were placed between the MWS and the backstop; one in front of the MWS (muzzle velocity) and the second close to the backstop (impact velocity). After perforation the speed of the projectile was determined with a double exposed picture of a digital camera (Figure 1), which is placed behind a PMMA window at one side of the backstop. The speed could be calculated from the time difference of two flashes (here: 0.1 ms) and the distance of the projectile within this time difference using the double exposed picture.

Based on the measured speed of the projectile and its known weight the kinetic energy before and after perforation could be calculated. Their difference corresponds to the energy necessary to generate the fracture particles and their kinetic energy following the impact.
As a consequence of the perforation a fractured surface area was created which consists of different parts. One part consists of the crater-area on the front and rear side of the specimen. The laser scanning system DAVID 3D was used to determine these surfaces. It is based on laser triangulation [3]. The setup of the laser scanning system consists of a line laser, a digital video camera (here a Sony DigiCam), a 90°-corner with a calibration pattern and the software DAVID. The principle arrangement of the measuring setup is given in Figure 2.

The line laser was installed in a small lift in order to assure reproducible test conditions. Thus, the laser went up and down and the intensity of the different scans was almost constant. The laser plane of the line laser intersects with the calibration pattern in the corner. In this study the calibration point distance for the camera was 300 mm and the surface smoothing operators for scanning and processing were used according to the recommendation of the manufacturer: interpolate = 4, smooth average = 2, and smooth median = 0. The new 3-dimensional coordinates of a single point are calculated by means of optical triangulation. As a result, the points scanned form a 3-dimensional point cloud defining the surface area, which then in turn can be calculated.
The second part of the fractured surface area is provided by the fragments which were disrupted from the specimens as a result of the projectile impact. Their surface area was determined using a computer particle analyzer (CPA) of Haver & Böker [14]. The CPA is based on digital image processing with a high-resolution digital line scan camera. It measures the shape-parameter sphericity, particle-size-parameters (Feret-diameter, length, volume distribution) and particle numbers of each size class analogue to a sieving analysis (following the sieving sequence R 20/3 of [15]).

A mathematical model is necessary to describe the surface area of the fragments. A sphere model was discarded for this purpose because the calculated volume of the particles as sphere was nearly two times higher than the measured volume (with: sphere-diameter = Feret-diameter). Thus, a triaxial ellipsoid model was chosen to determine the surface of the particles. By knowing two of three half axes of an ellipsoid (average Feret-diameter and average length of each size class) the third axis could be calculated by using the known volume V. The formula of Thomsen [16] for the surface area of the ellipsoid led to a good approximation. Additionally, a shape factor was developed which considered the particle-shape-parameter measured. The shape factor is defined as the quotient of the measured sphericity Circ and the sphericity CircE of an ellipse constructed of the measured Feret-diameter F and the length L. The surface area of each size class A_{SC} could be calculated by equation (1) where N_{SC} means the number of particles of this size class.

\[
A_{SC} = N_{SC} \cdot \frac{\text{Circ}}{\text{CircE}} \cdot 4 \cdot \pi \cdot \left( (F \cdot L)^{1.6} + \frac{3 \cdot V}{N_{SC} \cdot 4 \cdot \pi \cdot F} \right)^{1.6} + \frac{3 \cdot V}{N_{SC} \cdot 4 \cdot \pi \cdot L} \right)^{0.625}
\]

A part of the fragments surface was not created by the impact but comprises the original surface of the formwork. This part must be discounted from the total fragments surface in order to obtain the surface fractured only. Therefore, pictures of the front and rear side of the specimens were taken directly after the tests with a main focus on the crater. The software AutoCAD scaled these pictures to the needed size. Subsequently a polygon was drawn
enclosing the crater. The resulting area enclosed by the polygon represented the original surface of the fragments before impact.

The fractured surface area comprises the sum of all surfaces of each size class plus the surface of the craters minus the original surface of the specimens.

3 EXPERIMENTAL RESULTS

3.1 Masses

The mean weight of the specimens before impact \(m_{bp}\) was measured to approx. 11200 g. After perforation the weight of the specimens \(m_{ap}\) decreased differently dependent of the weight of the detached fragments \(m_f\). All masses are given in Table 3.

<table>
<thead>
<tr>
<th>Test series</th>
<th>(m_{bp}) [g]</th>
<th>(m_{ap}) [g]</th>
<th>(m_f) [g]</th>
</tr>
</thead>
<tbody>
<tr>
<td>875 m/s</td>
<td>11183 (0.010)</td>
<td>10830 (0.014)</td>
<td>327 (0.288)</td>
</tr>
<tr>
<td>710 m/s</td>
<td>11121 (0.015)</td>
<td>10864 (0.014)</td>
<td>237 (0.256)</td>
</tr>
<tr>
<td>605 m/s</td>
<td>11199 (0.026)</td>
<td>10955 (0.027)</td>
<td>228 (0.267)</td>
</tr>
</tbody>
</table>

3.2 Velocity and energy

The mean values of the measured velocities and the energy difference calculated are given in Table 4. The energy differences were calculated using the velocities before and after impact and assuming a constant mass of the projectile (9.5 g). In most cases the tungsten carbide core was not destroyed; thus, no energy was used for deforming the core. The energy differences rise with an increasing muzzle respectively impact velocity.

<table>
<thead>
<tr>
<th>Test series</th>
<th>(v_{impact}) [m/s]</th>
<th>(v_{after,perforation}) [m/s]</th>
<th>(\Delta E) [J]</th>
</tr>
</thead>
<tbody>
<tr>
<td>875 m/s</td>
<td>875.7 (0.005)</td>
<td>664.8 (0.054)</td>
<td>1538 (0.135)</td>
</tr>
<tr>
<td>710 m/s</td>
<td>710.3 (0.005)</td>
<td>484.5 (0.049)</td>
<td>1279 (0.087)</td>
</tr>
<tr>
<td>605 m/s</td>
<td>605.2 (0.005)</td>
<td>348.9 (0.103)</td>
<td>1156 (0.098)</td>
</tr>
</tbody>
</table>

3.3 Number of fragments and surface area

The number of fragments increases with a higher muzzle velocity and a smaller sieving width. Figure 3 shows the mean numbers of fragments of all test series dependent of their size. The diagram has a bi-logarithmic scale. The highest number of fragments during testing all three velocities can be found in the sieving class 0.125 / 0.18 mm. The sum of all
fragments varied between 1.94 million for 605 m/s and 4.17 million for 875 m/s. For a speed of 710 m/s 2.66 million fragments were measured.

**Figure 3**: Number of fragments in different sieving classes

The mean values of the sphericity of the fragments were in the same range irrespective of the impact speed. They vary between 1.21 (710 m/s) to 1.25 (605 m/s) and 1.26 (875 m/s).

The surface areas of the fragments were calculated from the values measured with the CPA. These surfaces are considerably greater than the corresponding crater surfaces. The mean sum of the surface areas of the front and the rear of each specimen detected with the laser-scanner was significantly higher for the highest muzzle velocity, but for the two other velocities the crater areas are more or less the same. All mean values and their coefficient of variation are presented in Table 5.

### Table 5: Surface areas (in parentheses: coefficient of variation)

<table>
<thead>
<tr>
<th>Test series</th>
<th>$A_{crater}$ [cm$^2$]</th>
<th>$A_{fragments}$ [cm$^2$]</th>
<th>$A_{original}$ [cm$^2$]</th>
<th>$A_{fractured area}$ [cm$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>875 m/s</td>
<td>213 (0.178)</td>
<td>4836 (0.085)</td>
<td>194 (0.274)</td>
<td>4855 (0.877)</td>
</tr>
<tr>
<td>710 m/s</td>
<td>166 (0.193)</td>
<td>3187 (0.117)</td>
<td>146 (0.200)</td>
<td>3207 (0.118)</td>
</tr>
<tr>
<td>605 m/s</td>
<td>167 (0.205)</td>
<td>2656 (0.109)</td>
<td>149 (0.195)</td>
<td>2674 (0.110)</td>
</tr>
</tbody>
</table>

### 4 DISCUSSION

The combined masses after perforation are marginally smaller than the masses before testing. The differences are about 0.2 % of the initial weights (but around 10 % of the
fragments weights). It can be assumed that all bigger fragments were found and measured. Thus, the loss of weight can be considered a loss of the finest fragments. This assumption is supported by the distribution of the number of particles (Figure 3). It could be expected that the number of fragments increases with a smaller sieving width, but it decreases for the finest measured sizes (< 0.8 mm). As a result the surface areas calculated are too small. This could be disregarded as long as different velocities are compared due to the fact that these mass losses occur in each of the test series.

The fractured surface area increases with a higher impact velocity, but a detailed analysis of different parts of it reveals a more complex situation. On one hand the area of the crater is almost equal for impact velocities of 605 m/s and 710 m/s while it differs for an impact velocity of 875 m/s. On the other hand the fragment area increases significantly with an increasing impact velocity as a result of the higher number of fragments, especially finer ones, created during the impact perforation. This situation shows the importance of a detailed fragment analysis. A simple measurement and evaluation of the crater surfaces only as it was done in earlier studies would result in misleading conclusions about the damage caused by impact.

As expected the energy of the projectile before and after perforating the specimens increases with the rising impact velocity. The interesting point is that the energy differences also increase with rising impact velocities. It is assumed that the energy difference consists of fracture energy to create fractured surface areas and kinetic energy to project the fragments out of the specimens. Thus, higher energy differences stand for more fracture energy and/or more kinetic energy of the fragments. The double exposed pictures show besides the projectile the maximum expansion of the fragment cloud. It reached almost the same speed as the projectile at that time. As a consequence the kinetic energy of the fragments increases with a higher impact velocity due to their higher speed and simultaneously their rise of masses. The higher fragment masses correspond with higher fracture areas. In order to create these areas more energy is consumed. Thus, the fracture energy increases also with higher impact velocities. This assumption is supported by fracture mechanical tests. Different studies show a rise of fracture energy when tested at higher speeds [17, 18, 19, 20]. One reason for this correlation could be seen in a higher strength and a higher deformability, but the exact explanation is not yet found.

Figure 4 shows the fracture surface areas and energy differences. The figure includes the mean values together with the minimum and maximum values of all test series. The Figure summarizes the question of this study: Does a higher muzzle velocity cause higher energy differences and an increased fracture surface area?
5 CONCLUSION AND OUTLOOK

In this study the damage on concrete specimen due to different impact velocities of projectiles were determined with special focus on the fracture surface area created. The marginal differences of the crater areas show that this criterion is insufficient to describe the damage. A thorough investigation must be based on measurements of all parts of the fractured area. Therefore a detailed fragment analysis is necessary. The largest part of the fracture area is provided by the surface of the fragments. These fragments are created by energy transformation. The kinetic energy of the projectile changed partial into fracture energy and kinetic energy of the fragments.

The two main conclusions of this paper are:
- Higher impact velocities lead to higher energy differences; thus, more kinetic energy of the projectile is absorbed and
- Higher impact velocities lead to higher fractured surface areas and hence a larger damage.

This knowledge can be used for designing concrete structures against impact. Future work will focus on different influences of concrete mix design upon impact perforation. Besides this, the energy parts within the energy differences have to be determined more closely.

REFERENCES


NUMERICAL SIMULATIONS OF GRANULAR MEDIA COMPOSED WITH IRREGULAR POLYHEDRAL PARTICLES: EFFECT OF PARTICLES’ ANGULARITY

E. Azéma∗, F. Radjai∗, F. Dubois∗

∗LMGC, CNRS-Universit Montpellier 2, Montpellier, France.
emilien.azema@univ-montp2.fr, frederic.dubois@univ-montp2.fr, franck.radjai@univ-montp2.fr

Key words: Granular Materials, particle shape, angularity, texture, force transmission

Abstract. We use contact dynamic simulations to perform a systematic investigation of the effects of particles shape angularity on mechanicals response in sheared granular materials. The particles are irregular polyhedra with varying numbers of face from spheres to “double pyramid” shape with a constant aspect ratio. We study the quasi-static behavior, structural and force anisotropies of several packings subjected to triaxial compression. An interesting finding is that the shear strength first increases with angularity up to a maximum value and then saturates as the particles become more angular. Analyzing the anisotropies induced by the angular distributions of contacts and forces orientations, we show that the saturation of the shear strength at higher angularities is a consequence of fall-off of the texture anisotropies compensated by an increase of the tangential force anisotropy. This is attributed to the fact that at higher angularity, particles are better connected (or surrounded) leading to an increase of friction mobilization in order to achieve the deformation. Moreover, the most angular particles also have very few sides so that, this effect is enhanced by the increase of the proportion of face-side and side-side contacts with angularity.

1 INTRODUCTION

One of the way to build a clearer picture of the complex behavior exhibited by real granular materials, is to understand and quantify the effects of grain shape. As shown experimentally and numerically by various author, angular[3, 7], elongated [4, 9] or non-convex [10] shapes, strongly affect the shear strength and the solid fraction, as well as the microstructure of the material. For example, they shows that this influence is sometimes counterintuitive, as in the case of the correlation between the elongation or the non-convexity of the grains and the solid fraction of the packing [4, 9, 10].

Nevertheless, a systematic and quantitative investigation of particle shape effect is still elusive because of three major difficulties: 1) Particle shape can be described in
terms of several parameters as angularity, elongation, flattening, non-convexity... 2) Each parameters need to be defined conveniently in order to be able to generate particle shapes with continuously-variables shape parameters; 3) Introducing grain shape in numerical simulations with discrete element methods gives rise to various technical difficulties both geometrical and computational as for example contact detection and force calculation between particles of arbitrary shape [5].

This work is dedicated more precisely to the effect of one of these parameters - angularity - on the mechanical behavior of sheared granular packings. We first introduce our numerical approach in section 2, then, in Sect. 3, the shear strength behavior is presented for different values of angularity. The microstructure is analyzed in terms of network connectivity and force transmission in sect. 4 and 5 respectively.

2 NUMERICAL PROCEDURES

The simulations were carried out by means of the contact dynamics method [1], which assumes perfectly rigid particles interacting through mutual exclusion and Coulomb friction. This numerical strategy, able to cope with stiff frictional contact laws, seems particularly relevant to address study of dense granular samples (even of large size) because it is not introducing numerical artifact due to contact stiffness. For this reason, the simulations can be performed with large time steps compared to molecular dynamics simulations. We used LMGC90 which is a multipurpose software developed in our laboratory, capable of modeling a collection of deformable or undeformable particles of various shapes by different algorithms.

Particles are constructed following a strict procedure in order to isolate and control precisely the shape. Firstly, a set of \( n_v \) vertex is randomly generated on the unit sphere. The convex hull of these points is created by associating three vertex for each faces. This condition imply that the number of face \( n_f \) is simply given by \( n_f = 2n_v - 4 \). Secondly, to be sure to avoid particle eccentricity, the degree \( \eta \) of distortion from a perfectly spherical shape, define as the ratio of the difference of the radius of subscribed and inscribed sphere over the radius of the subscribed sphere [9, 10] is computed. This parameter is similar to the Sphericity parameter used in soils mechanics. For nearly spherical particle we have \( \eta < 0.1 \). In other words, the first step is repeated until this condition was satisfied. We define thus the angularity \( \alpha \) of a particle as the mean angle between touching faces of the polyhedra. In this simple way, for a given aspect ratio, we can control the angularity of the particles with a single continuously-variable shape parameters depending only to the number of faces \( n_f \).

We prepare 6 different packings, named \( S_2 \) to \( S_7 \), each of them comprising 40,000 irregular polyhedra with the same number of faces \( n_f \) with \( n_f \in [176, 96, 46, 30, 20, 8] \). The packing angularity \( \langle \alpha \rangle \) is given by the mean angularity of the particles in the packing. In addition, we prepare a last packing \( S_1 \), composed of spheres. In order to avoid long-range ordering, we introduce also a small size polydispersity by varying the diameter of the sphere circumscribing the particles. Figure 1 displays snapshots of the packings for
two values of $\langle \alpha \rangle$ at the end of isotropic compaction presented below.

All samples were compacted by isotropic compression inside a box of dimensions $L_0 \times l_0 \times H_0$ in which the left, bottom and background walls are fixed and the top, the right and the front walls are subjected to the same compressive stress $\sigma_0$. The gravity was set to zero in order to avoid force gradients in the samples. The coefficient of friction was set to 0 between grains and walls during the isotropic compression. Thus, at equilibrium, all samples were in isotropic stress state. The isotropic samples are then subjected to vertical compression by downward displacement of the top wall at a constant velocity $v_y$ for a constant confining stress $\sigma_0$ acting on the lateral walls. The friction coefficient $\mu$ between particles is set to 0.5 and to zero with the walls.

3 MACROSCOPIC SHEAR STRENGTH

The stress tensor $\sigma$ can be evaluated from the simulation data as an average over all the contact of the dyadic product of contact force $f^c$ and branch vector $\ell^c$:

$$
\sigma_{\alpha\beta} = n_c \langle f^c_{\alpha} \ell^c_\beta \rangle_c
$$

[1], where $n_c$ is the number density of contacts $c$. Under triaxial conditions with vertical compression, we have $\sigma_1 \geq \sigma_2 = \sigma_3$, where the $\sigma_\alpha$ are the stress principal values. We extract the mean stress $p = (\sigma_1 + \sigma_2 + \sigma_3)/3$ and the stress deviator $q = (\sigma_1 - \sigma_3)/3$.

The principal strain values are

$$
\varepsilon_1 = \int_{h_0}^{h} dh'/h', \quad \varepsilon_2 = \int_{L_0}^{L} dL'/L' \quad \text{and} \quad \varepsilon_3 = \int_{l_0}^{l} dl'/l'.
$$

The cumulative shear strain is defined by $\varepsilon_q \equiv \varepsilon_1 - \varepsilon_3$.

Figure 2(a) shows the normalized shear stress $q/p$ as a function of shear strain $\varepsilon_q$ for all values of $\langle \alpha \rangle$. The shear stress jumps initially to a high value before decreasing to a nearly constant value in the steady state. The steady-state shear stress $(q/p)^*$ characterizes the shear strength of the material. According to the Mohr-Coulomb model, in tri-axial geometry, the internal angle of friction, representing the shear strength of the material, is defined by $\sin \phi^* = 3q/(2p + q)$ [6]. Interestingly, as shown by Fig. 2(b), the shear strength first increase with $\langle \alpha \rangle$ from 0.2 (spheres) and then saturate to $\approx 0.4$ for the most angular shape. The saturation of $\phi^*$ suggests that, as $\langle \alpha \rangle$ increases, important changes occur in the grain-scale phenomena underlying macroscopic friction.
4 CONTACT NETWORK CONNECTIVITY

The contact network can be characterized by the coordination number $z$ (average number of contacts per particle), which describe at the first order the connectivity of the packing. Figure 3(a) shows $z$ as functions of $\langle \alpha \rangle$ averaged in the residual state. We see that $z$ increase from 4 to 5 with $\alpha$ showing that for large angularities, the packings are better connected. This can be attributed to the fact that sharp corners and sides, for most angular particles facilitate contacts with close neighbors that would be unreachable for rounder particles. This can be evidenced plotting the proportion of face-face ($k_{ff}$), face-side ($k_{fs}$), side-side ($k_{ss}$) and face-vertex ($k_{fv}$) as a function of $\langle \alpha \rangle$; Fig.3(b).

We see that $k_{fv}$ decrease quickly from 1 (for spheres) to 0.15 with $\langle \alpha \rangle$. At same time, $k_{ss}$ increase nearly symmetrically from 0 to 0.6. The proportion of $fs$ contacts increases slightly to 0.2 whereas $k_{ff}$ pass by a pic equal to 0.2 before declines to nearly 0.05. In this way, as the particle angularity increases, the packing passes from a contact network dominated by $fv$ contacts to a contact network dominated by $ss$ and $fs$ contacts. The increasing connectivity of the particles is obviously correlated with the increase of shear strength due to the fact that face-side and side-side contacts are able to accommodate stronger forces chains than face-vertex contacts [7, 8].
Figure 4: (a) Snapshot of radial forces in packing for S4 in the steady state. Line thickness is proportional to the radial force (b) contact and forces anisotropies, as a function of $\langle \alpha \rangle$ in the residual state.

5 TEXTURE AND FORCE TRANSMISSION

Figure 4(a) shows a typical map of radial forces in granular media (here for S4) highlighting the peculiar organization of forces. The force chains are clearly inhomogeneous forming anisotropic structures generally at the origins of shear strength. To analyze this anisotropic structures, a common approach used by various authors is to consider the angular distribution of contacts orientations $\mathbf{n}$, as well as the angular average of normal and tangential forces along the direction $\mathbf{n}$. In 3D, let $\Omega = (\theta, \phi)$ the azimuthal and radial angles that define the orientations of $\mathbf{n}$. Under the axisymmetric conditions of our simulations, it is easy to see that each of this probability density functions are independent of the azimuthal angle $\phi$. Moreover, under shearing, the packing self-organizes into a state where a simple approximations based on spherical harmonics at leading terms captures their anisotropies [2, 8]:

$$
\begin{array}{ll}
\langle f_n \rangle(\theta) &= \langle f_n \rangle \{1 + a_c [3 \cos^2(\theta - \theta_c) - 1]\}, \\
\langle f_t \rangle(\theta) &= \langle f_n \rangle a_{ft} \sin 2(\theta - \theta_{ft}),
\end{array}
$$

(1)

where $\langle f_n \rangle$ is the mean normal force, $a_c$, $a_{fn}$ and $a_{ft}$ are the contact, normal force and tangential anisotropic parameters, and $\theta_c = \theta_{fn} = \theta_{ft} = \theta_n$ the privileged directions of the corresponding angular direction coinciding with the principal direction of the shear stress.

The anisotropies $a_c$, $a_{fn}$ and $a_{ft}$ are interesting descriptors of granular microstructure and force transmission properties, because they underlie the different microscopic origins of shear strength. Indeed, it can be shown that the general expression of the stress tensor leads to the following simple relation [2, 8]:

$$
\frac{q}{p} \simeq \frac{5}{2} (a_c + a_{tn} + a_{tt} + a_{fn} + a_{ft}),
$$

(2)

where $a_{tn}$ and $a_{tt}$ are the anisotropy of the mean orientation of the branch length projected along the normal and tangential direction, and where the cross products between the
anisotropy parameters have been neglected. In our simulation, due to the absence of shape eccentricity of the particles, we have $a_{tn} \sim a_{lt} \sim 0$. Figure 2(b) shows that Eq. 2 holds well for all values of $\langle \alpha \rangle$.

Figure 4(b) shows the variation of this three anisotropies as a function $\langle \alpha \rangle$. We see that $a_c$, $a_{fn}$, and $a_{ft}$, first increase with $\langle \alpha \rangle$, underlying the increase of the shear strength. This is a consequence of the increasing number of face-face, side-side and face-side contacts, which allow the force chains to be much more stable. Then, for $\alpha \gtrsim 0.5$ there is a decrease of $a_c$ compensated by a increase of $a_{ft}$ whereas $a_{f_n}$ remains constant, which explains the strength plateau shown in Fig. 2. This happens because very angular particles also have very few faces, so that it becomes difficult to orient these faces perpendicularly to the direction in which the forces are being transmitted. This causes the anisotropies $a_c$ to decrease. In addition, $a_{ft}$ increases, since the stability of such contacts relies on a strong activation of friction forces [8, 9, 10]. This is well illustrated in Fig. 5 where a map of mobilized forces (ie $f_t = \mu f_n$) are shown in red for S3 (a) and for S7 (b).

6 DISCUSSIONS AND CONCLUSIONS

In this paper, we applied the contact dynamics method to simulate large samples of polyhedral particles. The angularity of the particles is controlled by varying the number of the face of the polyhedra. It was shown that the shear strength first increases with the angularity and then remains nearly constant at larger angularity. For high angularities, the plateau of shear strength results from a decrease of the contact anisotropies compensated by an increase of the tangential force anisotropy. This transition results from a geometric effect that becomes dominant for very angular particles (a few number of faces along the stress direction) and that implies that the stability of the packing relies strongly on friction forces (particles are better surrounded).

Nevertheless, much more work is needed in order to understand the mechanical role of each contact type on the stress transmission. An idea is to isolate the contribution of each contact on the texture and forces anisotropies. On other way, a well known result
of idealized granular media is that the contacts can be classified into strong and weak networks with distinct mechanical role. It will be interesting to revisit this concept for our angular particles. This investigation are underway and they will be presented in forthcoming publication.

REFERENCES


STUDY OF THE CHARGING OF A BLAST FURNACE WITH A ROTATING CHUTE USING THE DISCRETE ELEMENT METHOD

MARK L. SAWLEY*, SAMI-ALEX ZAÏMI† AND DOMINIQUE SERT†

* School of Engineering (STI)
Ecole Polytechnique Fédérale de Lausanne (EPFL)
Station 11, CH-1015 Lausanne, Switzerland
e-mail: mark.sawley@epfl.ch

† ArcelorMittal Global Research & Development
Voie Romaine, F-57283 Maizières-lès-Metz, France
e-mail: sami-alex.zaïmi@arcelormittal.com, dominique.sert@arcelormittal.com

Key words: Blast furnace, discrete element method, size segregation, validation

Abstract. A numerical study of the charging process of a full-scale blast furnace, based on the Discrete Element Method, is presented. This study concentrates on the granular flow in a rotating chute employed to distribute appropriately the charge in the furnace. Detailed analysis of the results of numerical simulations has been undertaken to determine specific phenomena of importance to the charging process. Validation of the numerical results is obtained by comparison with experimental measurements of the position of the charge stream after exiting from the chute. The numerical results are shown to be in excellent qualitative and quantitative agreement with the experimental observations.

1 INTRODUCTION

A blast furnace is a large metallurgical device for the industrial production of iron.[1] The raw materials, iron ore and coke, are continuously introduced in particulate form at the top of the furnace, while pre-heated air is injected through tuyeres near the bottom. The charge material (or burden) descends in the furnace and, as a result of chemical reactions, is extracted as molten pig iron. A detailed understanding of this complex smelting procedure is essential for quality improvement of the resultant product. While blast furnaces have been used for many centuries, significant improvements have been made in recent years through better control of the different underlying processes.

The charging of the raw materials into a blast furnace is one of the critical operations governing the quality of the resultant product. For optimal operation, a burden comprised of consecutive layers of iron ore and coke with the desired radial distribution of ore/coke ratio is required to manage heat and chemical transfers within the core of the blast furnace. For this purpose, a variety of complex charging systems have been devised. To maintain precise control over placement of the charge, it is advantageous to replace the conventional bell system by a rotating semi-cylindrical chute. A chute has two rotational degrees of freedom – around the vertical axis (controlling the rotational speed) and about the horizontal axis.
(controlling the chute inclination) – that can be adjusted in an attempt to provide the ideal helicoidal charge distribution.

Numerical simulation has an important role to play in such a hostile environment where detailed measurements can be difficult to obtain. A number of previous numerical studies have examined different aspects of the smelting procedure. In particular, the Discrete Element Method (DEM) has been employed to study the charging process (e.g. [2-4]), and coupled to Computational Fluid Dynamics (CFD), the analysis of the burden movement throughout the blast furnace (e.g. [5-7]). While the excessively large number of particles in a blast furnace currently excludes complete full-scale DEM simulations, valuable insights have been gained through appropriate simplifications. Nevertheless, detailed validations of such results are required to assess their relevance and accuracy.

In this paper, a numerical study of a rotating chute charging system in the ArcelorMittal Dunkerque HF4 blast furnace is presented. DEM is used to simulate, under different operational conditions, the particle trajectories of a charge having an appropriate size distribution. Detailed qualitative and quantitative analyses of the numerical simulation results are presented, which provide insights into the charging process. Validation of the numerical results, obtained by comparison with experimental trials using painted bars to detect the position of the charge stream after exiting from the chute, is also presented.

2 PROBLEM DESCRIPTION

In a blast furnace, the iron ore and coke are generally individually loaded into the top of the furnace via a conveyor belt. For the HF4 blast furnace considered here, these raw materials are temporarily stored in two intermediate hoppers, which feed alternatively the rotating chute that distributes the iron ore and coke in successive layers at the top of the burden (Figure 1a).

The present study is focused on the behaviour of the particle flow due to the rotating chute, and hence a simplification of the charging system is considered. The upper section of the charging system is replaced by a centrally-positioned cylindrical hopper that feeds directly the rotating chute (Figure 2a). This enables a decoupling of the influence on the particle stream of its flow through the upper part of the charging system; while it is considered that this should not significantly affect the present results, confirmation would require an analysis based on numerical simulation results obtained using a more complete geometry.

Of particular significance to the present study is the design of the rotating chute. The chute employed in the HF4 blast furnace is comprised of a semi-circular trough of length 4.5 m and radius 0.55 m and rotates at a speed of 8 rpm. It contains attached brackets and lateral reinforcing support plates at regular intervals along the internal surface (Figure 1b). A description of the chute based on a detailed CAD representation was used for the numerical simulations. The actual height of the support plates was integrated into the numerical model although, for simplicity, only every second plate is represented (Figure 2b). Numerical simulations were performed both with and without the support plates. The throat of the blast furnace is represented by a cylinder of diameter 10.5 m.
Figure 1: (a) Schematic diagram of a bell-less charging system, and (b) photograph of the rotating chute and painted rods.

Figure 2: (a) Geometry used for the numerical simulations, with (b) a close-up of the rotating chute.
Only one fill material is considered in the present study, with properties corresponding to those of the coke charge. The particles are considered to be of spherical shape. The actual particle size distribution is approximated by a distribution comprised of five particles sizes, as shown in Table 1. The hopper contained initially 40,000 particles.

### Table 1: Particle size distribution

<table>
<thead>
<tr>
<th>Type</th>
<th>Diameter [mm]</th>
<th>Number fraction [%]</th>
<th>Mass fraction [%]</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>32.5</td>
<td>57.88</td>
<td>14.9</td>
</tr>
<tr>
<td>2</td>
<td>50</td>
<td>31.79</td>
<td>29.8</td>
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<tr>
<td>3</td>
<td>70</td>
<td>8.23</td>
<td>21.2</td>
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<tr>
<td>4</td>
<td>90</td>
<td>1.86</td>
<td>10.2</td>
</tr>
<tr>
<td>5</td>
<td>110</td>
<td>0.24</td>
<td>23.9</td>
</tr>
</tbody>
</table>

To enable validation of the numerical simulation results, the full-scale HF4 blast furnace was instrumented with painted rods (observed in the photograph in Figure 1b) at a distance of 5.14 m below the upper part of the chute (which corresponds to the lower edge of the hopper in the numerical simulations). The marking of these rods by the particles provides a quantitative measure of the radial position of the charge stream at this axial (vertical) location. Qualitative validation of the numerical simulations is also possible through comparison with photographs of the charge in the rotating chute taken during the operation of the blast furnace.

### 3 NUMERICAL METHOD

The numerical simulation of the charging of the blast furnace was performed using the Discrete Element Method. A soft-particle approach is employed, with collisions between particles and with the surfaces detected and the resulting normal and tangential forces and torques determined using a conventional linear spring-dashpot model.[8,9] The particles are assumed to be cohesionless, however, the effect of rolling resistance is taken into account. Although particle shape has been shown to play an important role in certain granular flows,[9] for the present study the particles were considered to be spherical.

The 3D surfaces of the blast furnace geometry are represented as a mesh comprised of triangular and quadrilateral elements. A rotational motion is imposed on the chute surface, while the other surfaces are stationary.

### 4 SIMULATION RESULTS

A number of DEM simulations were undertaken to gauge the parameters that play an important role in the particle flow behaviour along and at the exit of the rotating chute.

Initial simulations were performed both with and without the support plates on the internal surface of the chute. As shown in Figure 3, for a chute angle of \( \beta = 51.6^\circ \) (with respect to the furnace axis), a significant difference can be observed between the numerical results obtained for these two cases. Without the support plates, upon contact with the chute surface there is little build-up of material with the particles sliding freely downwards, retaining enough energy to rise up the curved side of the chute. The particles exit the chute with a sizeable kinetic energy, and are thus projected a substantial distance towards the furnace throat. With

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the support plates, the initial particles are locally trapped between the plates and form a bed onto which subsequent particles impact. Such impacts, as is well known from the granular flow literature, result in a substantial dissipation of the particles’ kinetic energy. Particles lose additional energy in traversing the length of the chute and are observed to remain located essentially at the bottom of the chute cross-section. This reduction in particle energy results in a significant modification of the particle trajectories on exit from the chute. The differences are observed to be greater for small chute angles $\beta$, due to the even lower loss of kinetic energy in the absence of support plates.

**Figure 3**: Particle motion within and on exit from the rotating chute for $\beta = 51.6^\circ$ and $t = 10$ s both (a) without and (b) with the support plates. (Particles are coloured according to their size.)
It is clear that the inclusion of the support plates into the numerical simulations is essential to analyse adequately the influence of the rotating chute. The plates are observed to play an energy-damping role, which governs strongly the particle trajectories on exit from the chute. It is noted that a damper plate has been incorporated into the chute designs studied by other authors [2,3] to provide a similar behaviour.

More quantitative results illustrating the above observations are provided in Figures 4 and 5, which present values averaged over the time period 4 s < t < 10 s for a chute at an angle of 51.6° and with support plates. Figure 4 shows the axial dependence of the average position of the particle stream and the normalized total (kinetic + potential) energy of the particles. These plots confirm a strong decrease in particle energy on contact with the particle bed that forms on the chute surface in the presence of the support plates. It is seen that more than half of the particles’ energy is lost while traversing the length of the chute.

![Figure 4: Time-averaged (4 s < t < 10 s) values of the axial dependence of (a) average radial position of the particle stream, and (b) total particle energy (β = 51.6°, with support plates).](image)

Figure 5 shows the mass-averaged radial distribution of the particle stream and of each of the 5 different component size types. Particle size segregation within the stream is evident, with the heavier particles being localized slightly further from the axis of the furnace. This behaviour is confirmed qualitatively by Figure 3, and appears to be produced by the tendency of the larger particles to be located near the upper surface of the flow within the chute.

Indicated in Figure 5a by the horizontal bar is the experimentally determined location of the particle stream at the axial position z = -5.14 m. The position of the particle stream on its exit from the rotating chute depends strongly on the interaction between the particles and the chute. Nevertheless, excellent agreement is observed between the numerical and experimental values of the stream location. Similar agreement has been obtained for each of the other 10 values of chute angle β considered in this study.
5 CONCLUSION

The results of the present study demonstrate that the Discrete Element Method is capable of simulating the particle dynamics associated with the charging of a full-scale blast furnace using a rotating chute. By accounting for the full complexity of the chute geometry, the location of the particle stream at its exit could be accurately predicted. Such confirmation of this numerical approach is an important initial stage for its integration into the industrial design process.

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REFERENCES


HUMAN BODAY DAMAGE ANALYSIS BY SPH METHOD

XUELONG LU*, HIROMASA KITAKAWA† TAKUYA MUKAI* YUZURU SAKAI*,

* Yokohama National University 79-1 Tokiwadai, Hodogaya-ku, Yokohama 240-8501 Japan
  e-mail: lu-xuelong-xg@ynu.jp
* Yokohama National University 79-1 Tokiwadai, Hodogaya-ku, Yokohama 240-8501 Japan
  e-mail: ysakai@ynu.ac.jp
* Yokohama National University 79-1 Tokiwadai, Hodogaya-ku, Yokohama 240-8501 Japan
  e-mail: s-fleet@cd6.so-net.ne.jp
† So-net Enterainment Coorporation 2-1-1 Osaki, Shinagawa-ku, Tokyo 141-6010 Japan

Key words: SPH, Particle Method, GPU volume rendering, CT image, Impact Problems.

Abstract. In order to evaluate the biological properties of a human head response at impacts accidents, authors have been developing the SPH (Smooth Particle Hydrodynamics) particle model of the whole human head and analyzing dynamically in simulating high velocity impact accident. In this report, authors have shown how to make a particle model of a head from real CT scan images directly and how to render the model in computer graphics using GPU and the algorithm for elastic-plastic analysis of a head model. The results from the simulations could explain one of injury mechanisms of a human head in actual car accidents.

1 INTRODUCTION

SPH (Smoothed Particle Hydrodynamics)[1-7] is a gridless Lagrangian technique which is promising as a possible alternative to numerical techniques currently used to analyze high deformation impulsive loading events, such as hypervelocity impact or explosive loading of materials, elastic-plastic analysis[8], heat transfer analysis[9] and other various phenomenon. While Eulerian techniques are appropriate to handle the gross motions associated with the large deformations, however detailed analysis is difficult because of the lack of history at the arbitral positions of the body by using Eulerian grid. Standard Lagrangian techniques are convenient to keep accurate histories of the events associated with each Lagrangian particles.

In general material models which describe the behavior of matter under extreme loading conditions usually require keeping precise histories at each material element or point. While it is relatively simple to produce this information from Lagrangian code calculations, it is a much more difficult task for an Eulerian code while Lagrangian techniques are excellent at tracking the history associated with each material point and can easily save the required information.

The basic SPH technique was first introduced by Lucy [1] and Gingold and Monahan [2] in 1977, and two comprehensive reviews are presented by Benz [3] and Monaghan [4]. More recently, the effect of strength was added by Libersky and Petschek [5], axisymmetric algorithms were developed by Johnson et al. [6], and Petschek and libersky[7].
In recent years, researchers have also shown the values of particle method for medical and biological analysis. Because the human body has complex geometries, it is very difficult to analyze by using mesh type models. Authors have confirmed the utility of a particle method for analyzing the structural problems of the human body. This study has been aimed to reproduce a human head particle model by using medical information (CT scanning data) and simulate the impact accident of a human head against a wall under high velocity (50 m/s).

2 ANALYSIS METHOD

2.1.1 Theory of SPH

The foundation of SPH is one of the interpolation techniques. The equation of motion and the conservation laws of substance, in the form of partial differential equations, are introduced into integral equations through the use of an interpolation function (weight function) that gives the estimate of the field variables at a point. In numerical process, information is given at discrete points, so that the integrals are evaluated as summing over neighboring particles. Figure 1 shows the concept of SPH method. Consider a function \( f \) and a kernel \( w \) which has a radius (support domain) \( h \), the kernel estimate is

\[
\int f(x')w(x-x',h)dx'
\]

As a typical weight function we employed the spline function of 3 degrees which is usually used in SPH analysis [10]. The approximation for spatial derivatives is obtained by substituting \( \nabla \cdot f(x) \) for \( f(x) \) in Eq. (1)

\[
\nabla \cdot f(x) \approx \nabla \cdot f(x')W(x-x',h)dx'
\]

In general physical parameters \( f(x) \) in a continuum is interpolated using a weight function and the discrete kernel estimate and its spatial derivative become
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\[ f(x) \approx \frac{1}{\rho} \sum_{j=1}^{N} m_j f(x_j) W(x-x_j, h) \]

And

\[ \nabla \cdot f(x) \approx -\frac{1}{\rho} \sum_{j=1}^{N} m_j f(x_j) \cdot \nabla W(x-x_j, h) \]

Where \( m \) is the mass, \( \rho \) is the density of the material and \( J \) is the interpolation points within a support domain. In this study, the elastic-plastic analysis is applied to human head impact against a rigid wall. The acceleration of a particle can be represented as follows using the stress divergence.

\[ a = \frac{1}{\rho} \nabla \cdot \sigma \]

Where \( \sigma \) is Cauchy stress tensor and \( a \) is acceleration. The acceleration of particle \( i \) is obtained as

\[ a_i' = -\frac{1}{\rho} \sum_{j=1}^{N} m'_j \sum_{j=1}^{3} \frac{\sigma_{ij}}{\rho^2} \frac{\partial W}{\partial x_j} \]

The variations of the Eq. (6) are sometime used. By using the stress tensor at point I, the Eq. (6) becomes

\[ a_i' = -\frac{1}{\rho} \sum_{j=1}^{N} m'_j \sum_{j=1}^{3} \left[ \left( \frac{\sigma_{ij}}{\rho^2} \right) + \left( \frac{\sigma_{ij}}{\rho^2} \right) \right] \frac{\partial W}{\partial x_j} \]

As the above equation, acceleration of any point in a stress field will be obtained. The interaction between Particle I and particle J is equal. That is, the law of conservation of momentum is guaranteed exactly.

Velocity gradient is given using Eq. (4)

\[ \left( \frac{\partial V}{\partial x_j} \right)_i = -\frac{1}{\rho} \sum_{j=1}^{N} m'_j V_j \frac{\partial W}{\partial x_j} \]

And

\[ \left( \frac{\partial V}{\partial x_j} \right)_i = \frac{1}{\rho} \sum_{j=1}^{N} m'_j (V_j - V_i) \frac{\partial W}{\partial x_j} \]

The latter relation has the advantage that the contribution to the strain rate tensor from particles I and J is zero if their relative velocity is zero. As Eq. (9), using the known particle positions and stress to seek acceleration at time \( t^n \), velocity and position is as follow.

\[ V_i^{t^n+\frac{1}{2}} = V_i^{t^n-\frac{1}{2}} + \frac{1}{2} \left( \Delta t^{n+\frac{1}{2}} + \Delta t^{n-\frac{1}{2}} \right) a_i^{t^n} \]
Particle density at time $t^{n+1}$ is

$$\rho(x) = \sum_{j=1}^{N} m_j W(x - x_j', h)$$  \hspace{1cm} (12)

Strain rate tensor is obtained by velocity gradient as follow equation.

$$\dot{\varepsilon}_{ij} = \frac{1}{2} \left( \frac{\partial V_j}{\partial x_i} + \frac{\partial V_i}{\partial x_j} \right)$$  \hspace{1cm} (13)

Vorticity tensor is obtained as

$$\omega_j = \frac{1}{2} \left( \frac{\partial V_i}{\partial x_j} - \frac{\partial V_j}{\partial x_i} \right)$$  \hspace{1cm} (14)

### 2.1.2 Artificial viscosity

In SPH analysis the discretization equation has inevitably numerical instability. To control the numerical instability, artificial viscosity terms are generally used. Just like the finite difference method, the artificial viscous stresses are given as follow equation.

$$Q = \rho b_1^2 \left( \frac{\dot{\rho}}{\rho} \right)^2 + \rho b_2 c \left( \frac{\dot{\rho}}{\rho} \right)$$  \hspace{1cm} (15)

Where $b_1$ and $b_2$ are length constant. $c$ is the sound speed. The artificial viscous stress is

$$Q = \rho b_1^2 \left( \frac{\dot{\rho}}{\rho} \right)^2 + \rho b_2 l^2 c \left( \frac{\dot{\rho}}{\rho} \right)$$  \hspace{1cm} (16)

Hence, equation of motion that containing artificial viscosity is

$$a_j = -\sum_{j=1}^{N} \sum_{i=1}^{3} \left[ \frac{a_j - Q\delta_{ij}}{\rho^2} \right] + \left[ \frac{a_j - Q\delta_{ij}}{\rho^2} \right] \frac{\partial W}{\partial x_j}$$  \hspace{1cm} (17)

As Monaghan pointed out follow equation, a common technique used is

$$Q^{ij} = \rho^2 \Pi^{ij}$$  \hspace{1cm} (18)

Where

$$\Pi^{ij} = \frac{\alpha C^{ij} \mu^{ij} - \beta (\mu^{ij})^2}{\rho^{ij}}$$  \hspace{1cm} (19)
2.1.2 Artificial viscosity

difference method, the artificial viscous stresses are given as follow equation. As Monaghan pointed out follow equation, a common technique used is

\[ \mu^u = \frac{h \sum_{j=1}^{N} (\mathbf{v}_j' - \mathbf{v}_i') \cdot (\mathbf{x}_j' - \mathbf{x}_i')}{{\|\mathbf{v}_j' - \mathbf{v}_i'\|}^2 + ch^2} \]

\[ C^u = \frac{1}{2} \left( C^i + C^j \right) \]

\[ \rho^u = \frac{1}{2} \left( \rho^i + \rho^j \right) \]

Thus,

\[ a^i_j = -\sum_{j=1}^{N} \sum_{j=1}^{m^i} \left[ \left( \frac{\sigma_{ij}'}{\rho^i} \right) + \left( \frac{\sigma_{ij}'}{\rho^j} \right) + \Pi^u \delta_{ij} \right] \frac{\partial W}{\partial \mathbf{e}_{ij}} \]

(23)

By using the above equation we can solve the impact analysis without the particle turbulent oscillations from the numerical instability.

2.1.3 Elastic-plastic analysis

SPH algorithm for elastic-plastic analysis method has been developed by authors. In the case that strain rate effects are not into account by using the elastic plastic algorithm in finite element analysis. In the finite element method, the yield judgment is performed at the numerical integration points of the element or the center point of element, while in SPH method yield condition is performed for each particle of the model.

SPH method used the yield condition which be applied in the finite element method. A typical expression of the Mises yield condition is the yield stress of material.

In this analysis we have used the Elastic-plastic problems always use deformation theory and incremental theory. SPH method interpolates explicitly, that easy to handle the incremental amount of physical expression. So authors use the incremental theory in elastic-plastic analysis too. In the elastic region

\[ \{d\varepsilon\} = \begin{pmatrix} d\sigma_x \\ d\sigma_y \\ d\tau_{xy} \end{pmatrix} = \frac{E}{1-v^2} \begin{pmatrix} 1 & v & 0 \\ v & 1 & 0 \\ 0 & 0 & 1-v^2/2 \end{pmatrix} \begin{pmatrix} d\varepsilon_x \\ d\varepsilon_y \\ d\gamma_{xy} \end{pmatrix} = [D_e] \{d\varepsilon\} \]

(24)

In the plastic region

\[ \{d\sigma\} = \begin{pmatrix} \frac{E}{1-v^2} S_1^2 & \frac{vE}{1-v^2} S_1 S_2 & -\frac{S_1 S_6}{S} \\ \frac{vE}{1-v^2} S_1 S_2 & \frac{E}{1-v^2} S_2^2 & -\frac{S_2 S_6}{S} \\ -\frac{S_1 S_6}{S} & -\frac{S_2 S_6}{S} & \frac{E}{2(1+v)} S_6^2 \end{pmatrix} \begin{pmatrix} d\varepsilon_x \\ d\varepsilon_y \\ d\gamma_{xy} \end{pmatrix} = [D_p] \{d\varepsilon\} \]

(25)

And stress-strain equation
\[ \sigma_y = D_y \varepsilon_y \]  

(26)

Used above equation authors can get the stress field.

3 PARTICLE MODELING

3.1 Title THREE DIMENSIONAL MODELING

To create computational models of the human head is placed polygon data in the boundary, or uses a three-dimensional voxel method to reconstruct CT/MRI medical images to particle models. Here authors use CT/MRI medical images brightness to arrange for the initial particle coordinates by voxel method.

In the past, to reconstruct a three-dimensional model by CT/MRI medical images often used unstructured grid to reproduce the complex geometry, could not represent a solid model. Authors use voxel data instead of polygon data. CT/MRI images are shot who ring-shaped by X-ray. Stacking height direction of ring-shaped slice images, make a three-dimensional model as figure 2. Slice images is quantized by brightness value than corresponding to each head tissue. Using threshold selection by the brightness value as a scalar, extract three-dimensional volume data = voxel. Authors used medical image brightness to create particle models directly, so the modeling is easy to apply in SPH method.

![Figure 2](image)

Figure 2 three-dimensional model

But in general, high-resolution medical images are often used, so the data will be enlarged. Authors have to select a required resolution. This time, authors used the discrete frequency conversion of wavelet analysis method to be applied to medical images, and extending to three-dimension, to create a model for SPH analysis.

![Figure 3](image)

Figure 3 Discrete wavelet transform to medical images

Used basic reference wave \( \psi(t) \) and scaled or moved in parallel to fit the input signal, reference wave \( \varphi_{j,k}(t) \) to transform.

\[ \varphi_{j,k}(t) = 2^{-j} \varphi(2^{-j}t - k) \]  

(29)
Here $\psi(t)$ used the simplest Haar Wavelet, the technique is like Figure 4. Authors reduced 512*512*512 resolution Three-dimensional images to any resolution images Figure 5. The compression trends will let original image to 1/512 Figure 6.

![Figure 4 3D Wavelet transform image.](image)

![Figure 5 Wavelet transform](image)

![Figure 6 the Wavelet transform compression trends](image)

### 3.2 Real Time GPU Rendring

Particle* volume data has a big problem that is data size too large. In this paper, authors used volume rendering on the GPU (Graphics Processing Unit), and can visualize experimental results in real time. Authors select two experimental methods. (1) Sampled texture on the GPU, the texture volume rending that can express property values based on the transfer function. (2) Sampled the particle data efficiently on GPU, ray casting in real time.

Texture rending is high affinity between GPU that easy to handle data of texture*color information. And also added rotation matrix to texture, always puts slice in the line of sight, to handle memory efficiently. Of course, polygons which map the particle data are used to cross each other with three-axis.

Ray casting is used in still image, it was not realistic to use in real time. Authors put volume on the GPU to take a sample, so ray casting allows real time processing. When the ray traverses the
volume, if it beyonds the scope of ray or opacity exceeding its threshold, then terminates the calculation.

Figure 7 Ray casting method image
This is a very useful technique for visualizing the internal state where in SPH visualizing. Both of follow, throughput speed is 30~75FPS. Processing in real time is confirmed.

Apply Marching cubes method to isosurface maintain continuity, cell cube next to each other reverse, turn polygon over, obtained normal vector by cross product, and normal vector reverse easily too. So authors added Split tetrahedron method to avoid normal vector reverse. Eq. (30) is determination of isosurface vertices.

\[
\vec{r}_n = \frac{n_0 - n_j}{(n_i - n_j)} (\vec{r}_i - \vec{r}_j)
\]

\(n\): density of volume, \(n_0\): density range, \(i, j\): grid \(r_s\): isosurface vertices coordinates

\[
\vec{\phi}_n = \frac{n_0 - n_j}{(n_i - n_j)} \vec{\phi}_j + \left(1 - \frac{n_0 - n_j}{(n_i - n_j)}\right) \vec{\phi}
\]

\(\phi\): normal vector of attracting attention grid

As follow image is 1 slice 512*512 pixel, be 0.3mm thick, 386 pieces CT data by discrete wavelet transform and compress volume, 108 polygons.
4 HEADINGS SPH ANALYSIS

As described modeling methods above, authors have been developed codes to make a human head computational model directly from CT/MRI images. The geometry of the model is based upon CT/MRI slices of a living human head and the particles represent an adult human head. Which has four parts: bones (include skin), brain, spinal fluid and meat tissue (include skin).

4.1 Analysis Condition

At first, authors made a simple model just had brain and bone.
Model: Brain: 35 million particles, bone: 15 million particles
Impact condition: impact orientation : front, angle : 75°, impact speed : 30m/s
Image just like Figure10.

The second Model: Brain: 289793 particles, bone: 67122 particles, spinal fluid and brain fluid: 106706 particles, skin and meat tissue: 363854 particles
Impact condition: impact orientation : front, angle : 75°, impact speed : 30m/s
4.2 SPH simulation result

Figure 11 is head impacted to wall and stress distribution.

Figure 12 is brain pressure transmission.

Figure 13 Stress transmission from front view.
4.2 SPH simulation result

Figure 11 is head impacted to wall and stress distribution. Figure 12 is brain pressure transmission. Figure 13 Stress transmission from front view.

Figure 14 precise model simulation result of brain pressure transmission. Stress is mises stress. Like the Figures showed collision parts had a large deformation and stress transmission clearly. Stress gradually is spread from outer to inside of brain. It has been observed high pressure occurs on the front of head when the impact from front or back. It is a match that is known, When traffic accident occurred, impacting from front to the head will be caused damage to the frontal region, impacting from back to the head will be caused damage to the front too.

Figure 15 precise model simulation result of stress transmission. The simple model’s pressure is transferred from front to back, but precise model’s pressure is difficult to transfer from front to back, are expected. The reason is the calculation added the brain fluid and spinal fluid which cushions, so pressure will be hard to transmission. And also need to change simulation conditions.
5 CONCLUSIONS

Authors addressed the problem of make a model from medical images directly, and simulate in high velocity impact of human head crash by SPH method. From now, authors need to make more precise human head model to assessment of human body injury (Include: fracture, retraction, amputate). And also authors must work for to apply SPH simulation and real time rendezing to three-dimensional virtual surgery (Include: dissection, ablation, bleeding).

Of course, in a traffic accident, head impact will come from any direction, authors need to calculate not only a head but also a man in the car or in other situation.

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REFERENCES

INFLUENCE OF POROSITY PERCOLATION ON MECHANICAL PROPERTIES OF CERAMIC MATERIALS.
3D SIMULATION USING MOVABLE CELLULAR AUTOMATA

ALEXEY YU. SMOLIN†, NIKITA V. ROMAN†, DARYA S. LOGINOVA†, IGOR S. KONOVALENKO* AND SERGEY G. PSAKHIE†

*Institute of Strength Physics and Materials Science (ISPMS)
Siberian Branch of Russian Academy of Sciences
pr. Akademicheskiy 2/4, 634021, Tomsk, Russia
e-mail: root@ispms.tomsk.ru, www.ispms.ru/

†Tomsk State University (TSU)
pr. Lenina 36, 634050, Tomsk, Russia
e-mail: rector@tsu.ru, www.tsu.ru

Key words: Porous Materials, Mechanical Properties, Computer Simulation, Movable Cellular Automata

Abstract. 3D computer simulation of mechanical behavior of a brittle porous material under uniaxial compression is considered. The movable cellular automaton method, which is a representative of particle methods in solid mechanics, is used for computation. In an initial structure the automata are positioned in FCC packing. The pores are set up explicitly by removing single automata from the initial structure. The computational results show that the curves of dependence of strength and elastic properties of the modeled specimens on porosity have a break at the porosity value about 20%, i.e. percolation threshold. The obtained results are in close agreement with available experimental data.

1 INTRODUCTION

It is well known that porosity dependence of strength and elastic properties of porous materials is determined by the pore morphology. If porosity is small, each pore is closed and isolated from the others. With porosity increasing the number of pores becomes greater and the distance among pores decreases. When porosity reaches percolation threshold the pores are not closed anymore and consequently form a new morphology. Thus, dependence of strength and elastic properties on porosity should be changed when percolation threshold is exceeded.
Note, it is very difficult to study the problem experimentally, because of stochastic nature of the pore morphology in real materials. For example, it is impossible to fabricate specimens with various porosity value and the same porous structure. At the same time potentialities of the modern computational mechanics allow to study in detail not only deformation of complex heterogeneous materials but also fracture of such materials.

2 COMPUTATIONAL MODEL FOR POROUS CERAMICS

For 3D computer simulation of mechanical behavior of a porous material under uni-axial compression we used the movable cellular automaton method (MCA) [1]. MCA is a method in discrete computational mechanics which allows modeling deformation and fracture of heterogeneous material with taking into account the structure of the material explicitly. Modeled material is represented as a set of elements of finite size (automata) interacting with each another according to some pre-determined rules. Mechanical interaction among automata are defined by so called response function, which can be interpreted as a local stress-strain diagram. Equation of translation motion and rotation of the automata are written in many-body approach. This means that interacting force between a couple of automata depends not only on position and state of these automata but also on position and state of their neighboring automata. This allows modeling as solid also as granular material behavior within the framework of one MCA method.

Response function of automata used in this study corresponded to ZrO$_2$ ceramics with average size of pores commensurable with the grain size of the material. According to the pore distribution diagram of this material [2] the automaton size in the computations was 1$\mu$m. All the modeled specimens where bricks with a square base. The loading was applied by assignment of vertical velocity for automata of the top layer of a specimen. At the same time the substrate automata were rigidly fixed. At the initial stage of the loading velocity of the upper automata increased by a sinusoidal law from 0 to 1 cm/s and then was constant.

Pores were generated by removing single automata from the basic structure. The porosity values were varied from 0 to 50%. Note, that the maximal porosity on the assumption of pore disconnection in closed packing of elements for 2D is $1/2 = 50\%$ (Fig. 1,a) while for 3D it is $1/4 = 25\%$ (in Fig. 1,b one closed packing plane is shown for FCC). In this

![Figure 1: Periodic pores (black) in closed packing](image-url)
case the pores are situated regularly.

The maximal value of closed porosity for random removing of single automata from FCC packing is 17.6%. The percolation limit for 3D FCC packing is 19.8%. Consequently, all the specimens used in this study with porosity greater than 20% contained clusters of interconnecting pores. For the specimens with porosity greater than 25% their porosity was interconnected.

In [3] it is shown that porosity structure defines not only elastic, but also strength properties of a material. The clusters of interconnecting pores present a new element of structure in addition to single closed pores. Thus, with porosity increasing the changes of elastic and strength properties of a material are expected after transition of the percolation limit.

3 DETERMINING THE REPRESENTATIVE VOLUME

At the first stage it is required to determine the representative volume of the modeled material. For material without pores the representative volume was determined based on four solid specimens. For this purpose the convergence of effective elastic modulus of the specimen $E_{\text{eff}}$ to the automaton elastic modulus $E_0$ with increasing the specimen size was analyzed.

The convergence was assumed to be satisfied if $E_{\text{eff}}$ differed from $E_0$ not greater then 3%. The computations showed the representative volume was equal 10 $\mu$m of the brick base size. The fracture pattern (cracks) in this specimen is shown in Fig. 2. The cracks are generated from the stress concentrators and propagate along maximum tangential stress direction.

![Figure 2: Fracture pattern of a solid ceramic specimen under compression: a) lines connect linked automata, b) lines connect unlinked automata](image)

If a material contains pores the cracks may initiate not in the corners but in the bulk
region of the highest local porosity. The direction of cracks propagation in such material is defined by the porous topology. Fig. 3 shows the first cracks in porous specimens with various values of porosity. One can see that the failure behavior of a porous material with large porosity and the failure of a solid material differs dramatically. In particular, the path of the crack propagation in porous material is rather crinkly.

![Figure 3: First cracks in specimens with various values of porosity C under compression](image)

The fracture pattern of the modeled brittle porous 3D specimens qualitative corresponds to 2D simulation results [3]. The quantitative difference is defined by the fact that porosity in 2D specimen is “interconnected” in the normal direction to the computational plane.

To analyze the dependence of elastic and strength properties of the modeled material on its porosity it is necessary to determine the size of representative specimen (volume). It is obvious that the representative volume for a porous material is different for different values of porosity. The simulations conducted show that for porosity value less then 15\% the representative volume is equal 20 \( \mu \text{m} \) (Fig. 4). For porosity value from 15 up to 35\% the size of representative volume is found to be 30 \( \mu \text{m} \) (Fig. 4,b). For porosity varied from 35 up to 50\% — 40 \( \mu \text{m} \) (Fig. 4,c).
Figure 4: Convergency of effective elastic moduli of the modeled specimens on their basis size for various porosity: a) 10%, b) 25%, c) 50%

4 STUDYING ELASTIC AND STRENGTH PROPERTIES OF POROUS CERAMICS

The loading diagrams of 3D modeled specimens are shown in Fig. 5. They are in close qualitative agreement with 2D simulation results [3, 4]. A quantitative difference between 2D and 3D results could be explained by the different influence of porosity on effective porous characteristics in 2D and 3D tasks.

First, it has to be noted that 3D specimens with porosity stochastically distributed in space can demonstrate quasi-viscous regime of fracture like 2D models [4]. To be able to failure in this regime the porosity of 3D specimens has to be greater than 40% (Fig. 5).

Let us consider dependence of the effective elastic modulus of 3D specimens on its porosity. In Fig. 6, a each square represents the value averaged on five representative specimens with various pore distribution in space. This plot obviously can be divided into two characteristic parts connected with porous structure: the first corresponds to closed
pores (5...20%), the second corresponds to clusters of interconnected pores (20...50%).
The experimental data taken from [2] are presented in Fig. 6,b for comparison. One can see the computational results are in close qualitative agreement with the experimental data. However, the inclinations of approximating lines showing degree of the influence of porosity on elastic characteristics of a material within the intervals are little bit different for the experimental and computational data. It can be explained by stochastic choice of elements for pore generation in the modeled specimens, and hence by the orientations of clusters of interconnected pores, which leads to reduction of porous structure influence on mechanical properties of a material. Besides, according to [2] percolation transitions in ceramics ZrO$_2$ cause microstructure change. In particular, internal stresses in ceramics with continuous porous structure restrain grain growth. Thus, simulation of uniaxial compression of brittle porous 3D specimens by the movable cellular automaton method showed that percolation transition from the closed pores to interconnected pores in a porous material leads to change in the dependence of its elastic properties on porosity.

Figure 6: Dependences of elastic modulus of ceramics on its porosity in logarithmic coordinates: a) simulation; b) experimental data

It is necessary to notice that this result could be obtained only in three-dimensional simulation because two-dimensional specimens with interconnected porosity are not topologically connected and do not resist to the mechanical loading. Besides, the porosity value at which formation of interconnected clusters occurs in a two-dimensional case (22.4%) is considerably less than the corresponding percolation limit (69.6%).

Fig. 7 shows the simulated and experimental dependencies of ceramics strength on its porosity. Again it can be divided into two characteristic parts connected with porous structure.
5 CONCLUSIONS

The simulations performed by the movable cellular automaton method show that the curves of dependence of strength and elastic properties of the brittle porous specimens on porosity have a break at the porosity value about 20%, which corresponds to percolation threshold. The obtained results are in close agreement with available experimental data.

In summary it is necessary to notice that for the purpose of the further application of the proposed 3D MCA model of porous ceramics it is necessary to extend the model with possibility of describing nonlinear properties of materials (degradation of elastic properties, relaxation at high-speed loading, etc.)

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MULTI-SCALE MODELLING OF DAMAGE PROGRESSION IN FRC LAMINATES – APPLICATIONS OF DEM

DONGMIN YANG*†, YONG SHENG*, JIANQIAO YE* and YUANQIANG TAN†

* School of Civil Engineering, University of Leeds, LS2 9JT, Leeds, UK
  Email: d.yang@leeds.ac.uk
  y.sheng@leeds.ac.uk
  j.ye@leeds.ac.uk

† School of Mechanical Engineering, Xiangtan University, 411105, Hunan, China
  Email: tanyq@xtu.edu.cn

Key words: FRC Laminates, DEM, Crack, Damage Progression.

Abstract. As a natural progress of the research in the area of modeling damage at microscopic scales, a discrete element method (DEM) has been proposed to simulate the damage progression in FRC laminates. DEM has been used to study the interfacial debonding, transverse cracking, delamination, and transverse cracking and delamination in FRC laminates. The purpose of this research is not only to validate the application of DEM in terms of its advantages in the simulation of damage progression and the prediction of cracking density and stiffness reduction, but also to highlight the potential of DEM in the future research application for composite damage mechanism, composite material design and optimization.

1 INTRODUCTION

Due to its superior properties, such as high strength, high stiffness and light weight, FRC has been widely used in engineering applications, particularly aerospace engineering, mainly as a replacement of conventional metals. Composite materials have shown excellent performances in the application of jet-engine by significantly increasing the thrust-to-weight ratios, compared with the traditional metal alloys. Fiber reinforced composite can fail in many different modes depending on the external loading conditions. For the prediction of composite failure strength and the purpose of composite product design, understanding of matrix, fiber and interface failure mechanisms is essential. These failure modes include fiber breakage, matrix cracking, debonding, delamination and eventually catastrophic failure [1]. The damage process of fiber reinforced composite is quite complicated because of the above damage types and more importantly the interaction between each other, especially under complicated loading conditions, for instance, triaxial loading or impact loading. Therefore it is necessary to treat the damage initiation and propagation in a progressive manner in a numerical model for composite damaging. The analysis and prediction of the progressive damage of composite is very challenging, but critical for the design and optimization of composite components for special applications.
To improve the understandings of damaging process in the fiber reinforced composite multi-ply laminates subject to static axial loads, a novel modeling methodology, Discrete Element Method (DEM) is presented to provide the advanced predictive capability and a computational tool that enables engineers to gain the insights of failure evolutions inside the material from microscale to macroscale so that designs can be optimized to enhance the damage tolerance of composite material.

2 DEM CONSTITUTIVE MODELS FOR COMPOSITE

DEM allows particles to be bonded together at contacts and to be separated when the bond strength or energy is exceeded. Therefore it can simulate the motion of individual particles and also the behavior of bulk material which is formed by assembling many particles through bonds at contacts with specific constitutive laws. In a DEM model of bulk material, elementary micro scale particles are assembled to form the bulk material with macroscopic continuum behavior determined only by the interaction of particles [2, 3]. Unlike the traditional solution using the strain and stress relations, contact properties are the predominant parameters in a DEM solution, combined with size and shape of the particles. Subject to external loading, when the strength or the fracture energy of a bond between particles is exceeded, flow and disaggregation of the particle assembly occur and the bond starts to break. Consequently, cracks form naturally at micro scale. Hence, damage modes and their interaction emanate as the process of debonding of particles. The way that DEM discretizes the material domain gives the most significant advantage over the traditional continuum mechanics based methodologies, as the difficulties encountered by the traditional methods, such as dynamic material behavior of composites, crack tip singularities and crack formulation criteria can all be avoided due to the naturally discontinuous representation for the microstructure of composite materials via particle assemblies in DEM.

Solid materials are usually modeled by DEM through adding a bond at the contact of two contacting particles. Bonds in DEM can be envisioned as a kind of glue joining the two contacting particles. There are two intrinsic bonds, contact bond and parallel bond in PFC2D [4] that is a popular commercial code of DEM and is used as the simulation platform of this research. A parallel bond can be regarded as a set of elastic springs with constant normal and shear stiffness, uniformly distributed over either a circular or rectangular cross-section lying on the contact plane and centered at the contact point [3]. Parallel bond can transmit both forces and moments, and will be used in this paper to describe the linear elasticity of fiber and elastic matrix. The parallel bond has a linear elastic behavior, as shown in Fig.1. The bond breaks when the contact force exceeds its strength [5, 6].

As suggested in [7, 8] that the interface between two composite plies is adhesive, there exist residual interfacial traction forces, even when the two plies are detached but before they are entirely separated. Therefore alternative contact models have been proposed by DEM users to account for the complex interfacial behaviour by considering more complicated constitutive laws. The contact softening model was proposed for this purpose based on the contact bond model [3, 9]. The concept of contact softening model (illustrated in Fig.2) is similar to the cohesive zone model (CZM) in the continuum mechanics [10, 11]. The only difference between these two models is the unloading and reloading curves after yielding.
The contact softening model describes the behavior of contact bonds in elastic, and represents plastic deformation by linearly softening the bond after the contact force reaches the bond strength. In both tensile and shear situations, the bond strength decreased to zero when the plastic displacement reaches the maximum plastic displacement \( U_{p,\text{max}} \) which is related to the fracture energy release rate \( G \). The interfacial crack may behavior as mode I, mode II or mix mode according to the stress field at the crack tip. In order to simulate the three fracture modes in DEM, the maximum plastic displacement \( U_{p,\text{max}} \) was kept constant, while the bond normal and shear strengths were defined individually. Hence, in a two dimensional system, the fracture energy release rate for mode I and mode II are, respectively:

\[
G_I = \frac{1}{2} \cdot \sigma_{n,\text{max}} \cdot U_{p,\text{max}}
\]

\[
G_{II} = \frac{1}{2} \cdot \sigma_{s,\text{max}} \cdot U_{p,\text{max}}
\]

The fracture energy release rate for mix mode can be calculated as:

\[
G = \frac{1}{2} \cdot \sigma_n \cdot U_p^n + \frac{1}{2} \cdot \sigma_s \cdot U_p^s = \frac{1}{2} \cdot \sigma_n \cdot \sum |\Delta U_p^n| + \frac{1}{2} \cdot \sigma_s \cdot \sum |\Delta U_p^s| (3)
\]

\( \sigma_n \) and \( \sigma_s \) are the normal and shear stresses of the bond when yield occurs. For the mixed mode, the fracture energy release rate is somewhere between the rates of two single fracture modes.
3 MODELLING RESULTS AND DISCUSSIONS

The damage behavior of DEM model depends on bond properties and particle size which have to be calibrated through virtual tension (or compression) tests as well as convergence tests before being used in the final models of composite. Details of model calibration are referred to our previous work in [5, 12-14], while only a summary of the DEM applications in modelling of composite damage progression, which covers matrix cracking, interfacial debonding, delamination as well as transverse cracking, is presented here.

The DEM modelling started with the simulation of material failure process in the microbond test of single fiber reinforced composites to investigate how the matrix cracks initiates and propagates to cause the fiber/matrix interfacial debonding, as shown in Fig.3. The plastic deformation and the cracking of the matrix were simulated by introducing the contact softening model. The initiation and propagation of interfacial debonding were captured naturally by the DEM simulation. Vises with two different vise angles were used in the simulations. It was found that the vise angle had effects on the material damage process [5].

![Fig.3 DEM simulation of micrbond test at different vise angle φ: (a) φ=7º, and (b) φ=14º.](image)

(Black dot indicates the bond has started to yield, and red dot indicates the final failure.)

DEM was then employed to simulate transverse cracking in composite laminae, due to its intrinsic advantages in modeling microscopic damage and fracturing in multiphased materials. Three types of fiber distributions, i.e., rectangular, hexagonal and random distributions, have been simulated to study the effect of fiber distribution on the transverse cracking, as
illustrated in Fig.4. The initiation as well as dynamic propagation of transverse cracking has been captured by the DEM model, showing good agreement to the experimental observations. Furthermore, the DEM simulations have provided unique insights of the microscopic cracking and damage in forms of matrix plastic deformation and fiber/matrix interface yielding. The effect of fiber volume fraction was also studied by using different fractions in the DEM modeling for randomly distributed fibers [14].

Fig.4 DEM dynamic simulation of transverse cracking in laminae

(*‘a’, ‘b’ and ‘c’ represent rectangular, hexagonal and random distribution of fibers, respectively; Red, black and brown lines describe transverse cracking, matrix plastic deformation and interface yield, respectively.*)
This work has further led to the findings that the distribution and volume fraction of fibers not only affect the transverse cracking path, but also the mechanical behaviors of the material through the populations of the residual matrix plastic deformation and fiber/matrix interfacial yielding.

To simulate initiation and propagation of delamination in anisotropic fiber reinforced composite laminates, a DEM model was developed by constructing a hexagonal arrangement of particle elements where contacts between particles were represented by parallel bonds with particular normal and shear properties. The contact softening model was introduced to count for the residual interfacial tractions. DCB, ELS and FRMM tests were simulated by the developed DEM model. Schematic in Fig.5 demonstrates a DEM model of DCB test in terms of crack evolution. Numerical results of loading curves were compared and found agreed very well with results from other numerical methods and experimental investigations. It has been confirmed that the present DEM model can simulate composite delamination accurately in all three fracturing modes with the capture of crack extension and plastic zone (see Fig.6) by which the complexity of dealing with the singularity at crack tips and the closing of existing cracks were all avoided [13].

Fig. 5 Schematic of damage propagation in DEM modelling of DCB test

Fig.6 Plastic zone and damage extension in DCB test

The initiation and propagation of transverse cracking as well as interfacial delamination in cross-ply laminates under uniaxial loading was eventually modelled by DEM. The 90° and 0°

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plies were respectively treated as isotropic and orthotropic materials whose elastic properties were accounted by adopting the parallel bond model at the contacts of the discrete particles. The interface between the 90° and 0° plies was represented by a contact softening model. The developed DEM model was validated by comparing the stresses distribution in a representative element of cross-ply laminate with the results obtained from the analytical methods. As an application of the developed DEM model, the transverse cracking and interfacial delamination in both $[0°/90°]_s$ and $[90°/0°]_s$ cross-ply laminates under transverse loading were analyzed by comparing the calculated crack density with the experimental data and other numerical predictions. The modelling result of $[0°/90°]_s$ cross-ply laminate was selected and shown in Fig.7 as an example. The comparisons shown that the DEM model is capable of not only modeling the damage in laminates at microscopic particle level, but also capturing both the transverse cracking and delamination phenomenon, and predicting crack density as well as stiffness reduction quantitatively at macroscopic level [15].

![Figure 7](image.jpg)

(a) $\sigma_c=64.38\text{MPa}$
(b) $\sigma_c=110.4\text{MPa}$
(c) $\sigma_c=294.3\text{MPa}$ (without interfacial delamination)
(d) $\sigma_c=294.3\text{MPa}$ (with interfacial delamination)

Fig.7 Dynamic initiation and propagation of transverse cracking and/or delamination in $[0°/90°]_s$, cross-ply laminate.

(Particles with blue and gray colors indicate 0° and 90° plies, respectively. Red short lines are micro-cracks in 90° ply, and black short lines indicate interfacial delamination.)

4 CONCLUSIONS

DEM has been used in the modelling of interfacial debonding, transverse cracking, delamination, and transverse cracking and delamination in FRC laminates. The outcome of this research has validated the application of DEM in composite laminates in terms of its advantages in the modeling of damage progression and the prediction of cracking density and stiffness reduction, and also proved the potential of DEM in the future research of composite material design and optimization.

REFERENCES

ON THE VALIDITY OF THE CARMAN-KOZENY EQUATION IN RANDOM FIBROUS MEDIA

K. YAZDCHI, S. SRIVASTAVA AND S. LUDING

Multi Scale Mechanics (MSM), Faculty of Engineering Technology,
University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands
e-mail: k.yazdchi@utwente.nl, http://www.utwente.nl/ctw/msm/

Key words: Fibrous Materials, FEM, Permeability, Microstructure, Carman-Kozeny relation.

Abstract. The transverse permeability for creeping flow through unidirectional random arrays of fibers/cylinders has been studied numerically using the finite element method (FEM). A modified Carman-Kozeny (CK) relation is presented which takes into account the tortuosity (flow path) and the lubrication effect of the narrow channels. The proposed relation is valid in a wide range of porosities compared to the classical CK equation. The proposed general relationship for the permeability can be utilized for composite manufacturing and also for validation of advanced coarse models for particle-fluid interactions.

1 INTRODUCTION

Fibrous materials are widely used in industry as well as our daily life due to their flexibility, strength, and most importantly, permeability [1]. One of the common examples of such materials is unidirectional fibre reinforced composites. These composites consist of a large number of 2D uni-directional fibres/cylinders embedded in the matrix phase at random locations perpendicular to the transverse plane. The goal is to determine the overall behaviour (i.e. mechanical and/or transport properties) of such a material provided that material properties and geometry of the matrix and fibres are known.

In most of the composite manufacturing processes (e.g. resin transfer moulding (RTM), autoclave process, vacuum infusion, etc.), the permeability is critically important. During the last decades, several researchers tried to develop a simple model that could predict the permeability of the fibrous medium as a function of solid volume fraction by incorporating computational/numerical or experimental measurements, see for example [1-5] and references therein.

In this respect, two distinct approaches have emerged; (i) the lubrication approach for dense systems and (ii) the cell method valid at larger porosity (dilute regime). Based on the lubrication theory at high volume fraction, the pores of a porous medium can be considered as a bunch of capillary tubes which are tortuous or interconnected in a network. An expression for the permeability as a function of solid spacing, for regular fibre arrays, was derived which closely matches the numerical results at high volume fractions [6-7].

On the other hand, for dilute systems, i.e. at high porosities, the cylinders are widely spaced, and the cell method is appropriate. It assumes that the cylinders are spaced far away so that the region can be divided into practically independent cells. Thus, the arrangement and
shape of the fibres has no effect on the permeability. In fact, at this limit, the permeability can be obtained by adding the resistance of individual particles/fibres. The dependence of permeability in this limit involves logarithmic, linear and quadratic functions of the solid concentration [8-10].

The earliest and most widely applied models in the composites literature, in intermediate porosity regimes, for predicting permeability are capillary models such as the Carman-Kozeny (CK) equation for random sphere packings [11]. While some studies have reported success with this relation, discrepancies are also reported. Gutowski et al. [12] found that the Carman-Kozeny equation could give a good fit to the axial permeability of unidirectional reinforcements, while there was a certain deficiency for the transverse permeability. It turns out that for the permeability prediction, the geometrical arrangement of fibres must be taken into account [13]. Although most parameters in this model can be calculated based on the geometrical structure of fibre reinforcements, it also has an empirical constant (the CK coefficient) determined by experimental data that can not be used directly for other types of fibre reinforcements.

In a recent work [14] the trend from low to high porosity extremes for regular structures is described, however, there is a lack of correspondence in the intermediate range of porosity for disordered fibre arrays. It is mainly due to difficulties in analyzing the precise geometry and topology of the pore system and proper characterization of the stochastic nature of the pore structure.

Our objective in this paper is to present a finite element based model that allows utilizing real 2D/3D microstructures in calculating the permeability of the fibrous materials. The macro description of the fluid flow equations and the numerical tools employed to solve these equations, are presented in the next Section. The permeability values obtained from our numerical results are compared with previous theoretical and numerical data for random and ordered configurations in Section 3. We propose a modification to the original CK equation as an attempt to combine our various simulations in a wide range of porosity and relate macroscopic permeability to the micro properties and geometry of fibrous materials. The paper is concluded in Section 4 with a summary and outlook for future work.

2 MATHEMATICAL FORMULATION

In this Section we summarize the relations describing the macroscopic flow in fibrous structures and the finite element method (FEM) employed to solve these equations.

2.1 Macroscopic description of the flow equations

The flow description in the porous media is based on the assumption that a Newtonian and incompressible fluid flows under steady-state conditions. The Navier-Stokes (NS), i.e. the conservation of momentum and the continuity equations, i.e. mass conservation, for this case reduce to

\[ \nabla \cdot \bar{u} = 0, \]

\[ \rho \left( \bar{u} \nabla \bar{u} \right) = -\nabla p + \mu \nabla^2 \bar{u}. \]  \hspace{1cm} (1)
where \( \mathbf{\bar{u}} \), \( \rho \), \( \mu \) and \( p \) are velocity, density of the fluid, viscosity and pressure of the fluid, respectively. When \( \rho \) and \( \mu \) are picked for a given fluid, solution of the flow problem yields the velocity profile for a given pressure gradient \( (\nabla p) \) which is applied as a boundary condition. This information is used to calculate the superficial velocity \( \bar{U} \), through the system as

\[
\bar{U} = \frac{1}{V} \int \mathbf{\bar{u}} dv \epsilon = \mathbf{\bar{u}} \epsilon
\]

(2)

where \( \langle \mathbf{\bar{u}} \rangle \), \( V \), \( V_f \) and \( \epsilon = V_f/V \) are the averaged velocity, total volume, volume of the fluid and porosity, respectively. According to Darcy’s law for unidirectional flow through a porous medium in creeping flow regime, the superficial fluid velocity is proportional to the pressure drop per unit length \( (\Delta p/L) \). The proportionality constant being the permeability \( K \), of the medium

\[
\bar{U} = -\frac{K}{\mu} \nabla p
\]

(3)

which strongly depends on the microstructure (e.g. fiber arrangement, void connectivity and inhomogeneity of the medium) and also on porosity. The effect of several microstructural parameters such as fiber shape, orientation, etc. in both creeping and inertial flow for regular structures have been studied in Refs [14-16] and references therein. In the next Subsection the permeability results obtained from FEM simulations for random fiber configurations will be presented.

### 2.2 Computational method

The FEM software ANSYS® is employed to calculate the superficial velocity and, using Eq. (3), the permeability of the fibrous material. Several issues like the required system size (or number of fibers), random packing generation algorithms, isotropy and heterogeneity of the structure were addressed in [17]. For all of our simulations presented here, we use the Monte Carlo (MC) procedure to generate random fiber structures. All simulated domains contain 800, non-overlapping fibers with minimum inter fiber distance \( \delta_{\text{min}}=0.05d \), where \( d \) is the diameter of the fibers.

Fig. 1 shows a schematic of a 3D and 2D representation of 200 randomly distributed fibers normal (y) to the flow direction (x) at porosity \( \epsilon=0.6 \) with minimum inter fiber distance \( \delta_{\text{min}}=0.05d \). Similar to Chen and Papathanasiou [3], a minimum distance is needed to avoid complete blockage. At the left and right boundary pressure is prescribed, at the top and bottom wall (z direction) surfaces and at the surface of the particles/fibers no-slip boundary conditions are applied. Fibers are assumed to be very long so that a 2D solution is representative. A typical unstructured, fine, triangular FEM mesh is also shown in Fig. 1. The mesh size effect is examined by comparing the simulation results for different resolutions (data not shown here). The range of number of elements is varying from \( 5 \times 10^5 \) to \( 10^6 \) depending on the porosity regime. The lower the porosity the more elements are needed in order to resolve the flow between close, neighboring fibers. To obtain good statistical accuracy, the permeability values were averaged over 10 realizations. Some more technical details are given in Refs [14, 17].
Figure 1: Fiber distributions generated by a Monte Carlo (MC) procedure, with 200 uni-directional cylinders, normal (y) to the flow direction (x), with minimum inter fiber distance $\delta_{\text{min}}=0.05d$ ($d$ is the diameter of the fibers) at porosity $\varepsilon=0.6$. At the top 3D and bottom 2D representation of the fiber distribution is shown. The zoom shows the fine, unstructured, triangular FEM mesh.

3 MODEL DEVELOPMENT AND NUMERICAL RESULTS

The earliest and most widely applied approach in the porous media literature for predicting the permeability involves capillary models such as the one that leads to the Carman–Kozeny (CK) equation [11]. It is based on Poiseuille flow through pipe and is mainly used for 3D, homogenous, isotropic, granular porous media at moderate porosities. In the next Subsections, we present a modified CK equation which takes into account the microstructure of the fibers and is valid in a wide range of porosities.

3.1 Permeability calculations

In the CK model [11], the hydraulic diameter $D_h$, is expressed as a function of the measurable quantities porosity and specific surface area

$$D_h = \frac{4\varepsilon V}{S_v} = \frac{4\varepsilon}{(1-\varepsilon)a_v} = \frac{\varepsilon d}{(1-\varepsilon)}, \quad \text{with } a_v = \frac{\text{particle surface}}{\text{particle volume}} = \frac{S_v}{(1-\varepsilon)V} = \frac{4}{d}$$

(4)

with the total wetted surface, $S_v$, and the specific surface area, $a_v$. The above value of $a_v$ is for circles (cylinders) – for spheres one has $a_v=6/d$. By applying the Poiseuille equation in terms
of the hydraulic diameter as $\langle \bar{u} \rangle = -\frac{D^2}{32 \mu} \nabla p$ and combine it with Darcy’s law, Eq. (3), the normalized permeability is

$$\frac{K}{d^2} = \frac{\epsilon^3}{\psi_{CK} \left(1-\epsilon\right)^2}$$

where $\psi_{CK}$ is the empirically measured CK factor which represents both the shape factor and the deviation of flow direction from that in a duct. It is approximated as $\psi_{CK}=180$ for random packed beds of spherical particles. Reported values of the CK factor for fibrous media are varying between 80 and 320 [18, 19]. The same range of $\psi_{CK}$ has been obtained from the theoretical results of Sangani and Acrivos [9]. Since their model was primarily developed for isotropic, granular porous media of spherical particles at moderate porosity, it is necessary to re-visit and modify the model for fibrous structures composed of arrays of cylinders.

The principal limitation of the CK equation is the fact that all geometrical features of the preform are lumped into the CK factor. Even though attempts have been made to introduce microstructural features of the preform into the CK equation by suitably modifying the mean hydraulic radius, it is fair to say that, at this stage, microstructural features can be included only semi-empirically through experimental determination of $\psi_{CK}$. An initial attempt was made by Carman [11] who considered the effect of flow path (tortuosity) on $\psi_{CK}$. Writing the CK factor in terms of its components, namely the pore shape factor $\Phi$ and tortuosity $L_e/L$,

$$\psi_{CK} = \Phi \left(\frac{L_e}{L}\right)^2$$

and combine it with Eq. (5), leads to

$$\frac{K}{d^2} = \frac{\epsilon^3}{\Phi \left(\frac{L_e}{L}\right)^2 \left(1-\epsilon\right)^2}$$

In the original CK equation it was assumed that the tortuosity is constant ($L_e/L = \sqrt{2}$) and $\Phi=90$, which gives us the CK factor as $\psi_{CK}=180$. However, in the next Subsection we will show that the tortuosity is not constant and linearly depends on the porosity.

### 3.2 Measurement of the tortuosity ($L_e/L$)

Along with porosity, tortuosity is one of the parameters that takes into account the influence of complex microstructure on the macroscopic permeability. It is defined as the average effective streamline length scaled by the system length, $L_e/L$, and turns out to be a key parameter in the CK factor [11]. Experimental data for tortuosity are obtained by the measurement of the effective diffusivity [20], effective conductivity [21], acoustic wave propagation [22], and permeability [23]. The obtained values are usually model dependent and restricted to beds of spheres. Depending on factors such as packing arrangement, media homogeneity, channel shape, etc., tortuosity values in beds packed with non-uniform spheres may range from 1.7 to 4 [24]. Correlations and analytical models for tortuosity are derived from geometrical considerations on the particle scale, and usually relate the tortuosity to porosity [25]. However, they are typically restricted to spherical particles. To obtain tortuosity
from our numerical simulations, we extract the average length of several streamlines (using 8 equal mass flux streamlines which divide the total mass in-flux into 9 zones, thus avoiding the centre and the edges). The tortuosity values are plotted in Fig. 2 as a function of porosity together with the best (least square) linear fit function. The tortuosity linearly depends on the porosity (with the slope of \( \approx 0.5 \)) at the intermediate porosity regime \((0.5<\varepsilon<0.95)\). Since in the limit of \(\varepsilon=1\) (no particles) one should approach the slab flow, i.e., \(L_c/L=1\), the linear fit is not accurate in the very dilute regime \((\varepsilon>0.95)\). By decreasing the porosity the standard deviation of the data (error bars in Fig. 2) increases which is an indication of non-homogeneity of the flow. In conclusion, we observe that (i) the tortuosity is not constant (linearly depends on porosity) and (ii) the value is smaller than \(\sqrt{2}\) for uni-directional random fiber arrays for all relevant, accessible porosities.

Knowing the values of \(L_c/L_c\), we have fitted our numerical results into Eq. (7) to obtain new pore shape factor \(\Phi\approx140\) within the range \(0.4<\varepsilon<0.9\). The proposed fit, based on the modified CK theory, matches the numerically calculated permeability with a maximum of 5% error in the porosity range \(0.4<\varepsilon<0.9\), applicable in most composite materials. In Fig. 3 the numerical results for the normalized permeability obtained from our FEM simulations in the wide range of porosity is shown. The comparison with the available theories, namely original CK \(\psi_{CK}=180\), the modified CK \(\psi_{CK}=140(L_c/L^2)\), the results of Drummond et al. [9] based on the cell method valid at high porosity, the analytical prediction of Gebart [10] based on lubrication theory valid at low porosity, both for the hexagonal configuration, and numerical results of Chen and Paphathanasiou [26] obtained from boundary element method (BEM) also displayed. For dilute systems, i.e., \(\varepsilon>0.9\), the permeability data obtained from the cell approach for regular structures [9] agrees well with our numerical results. Therefore, we
confirm that at high porosities, the effect of structure vanishes. At moderate porosities, i.e., $0.4<\varepsilon<0.9$, the proposed modified CK equation fits better to our FEM results. However, at low porosity, i.e., $\varepsilon<0.4$, none of the models fit to our FEM results. This observation can be explained by looking at the microstructure (local fiber arrangement) and orientation of the narrow channels. Fig. 4 shows the distribution of the orientation of the channels $\theta$, with respect to the flow direction, at different porosities.

![Figure 3: Comparison of normalized permeability as a function of porosity for (dis)ordered fibrous media. $\psi_{CK}$ is the Carman-Kozeny factor. $K^h_G$ and $K^h_D$ represent the lubrication theory of Gebart [6] and the unit cell approach of Drummond and Tahir [8] both for hexagonal configurations, respectively.](image)

![Figure 4: Plots of the probability density function (PDF) of the orientation of narrow channels at different porosities. On the right, the top shows the perfect hexagonal structure and the bottom graph, shows the schematic of the frequent hexagonal structure seen at low porosity ($\varepsilon=0.3$).](image)
At high porosities we observe isotropic distributions of orientations (circular shape in red and black color in Fig. 4). However, at low porosities we see higher probabilities at 30°, 90°, 150° etc., indicating localized crystal (hexagonal) structures. In other words, in this limit we have ordered hexagonal structures which are rotated by 30° with respect to flow direction. The distribution of these orientations shows that they are more directed in vertical direction. Note that for \( \varepsilon < 0.4 \) the effect of finite size and rigid walls/boundaries are more pronounced [17] and one might need just periodic, or much bigger systems (and/or more fibers/realizations) to obtain reliable random system and permeability data. However, the proposed modified \( \psi_{CK} = 140(L_c/L)^2 \) is still closest to our numerical results for intermediate porosity.

4 CONCLUSIONS

A finite element based model has been employed to calculate the transverse permeability of fibrous media composed of randomly distributed long unidirectional cylinders/fibers in wide range of porosities.

It is shown that the semi-analytical Carman-Kozeny (CK) equation does not correctly capture the permeability’s dependence on porosity. Therefore, an alternative relation for the permeability of the medium, taking into account the tortuosity (flow path) is developed from our numerical (FEM) results. We propose a CK coefficient, which is defined as the product of tortuosity (flow path) and pore shape factor \( \Phi \), for the intermediate porosity regimes. The modified CK equation with the new CK coefficient fits better to our numerical results in the moderate porosity range. Our results indicate that the tortuosity linearly depends on the porosity with the slope of \(~0.5\) (see Fig. 2). At high porosities \( \varepsilon > 0.9 \), the random and regular configurations predict the same permeability, i.e., the effect of structure will disappear. However, at low porosities \( \varepsilon < 0.4 \), the permeability data is lower than the values obtained from lubrication theory for hexagonal configurations and the proposed fit, based on the modified CK theory. This can be explained by looking at the microstructure and local arrangement of particles/fibers (see Fig. 4).

The results obtained in this study and the modified CK relation proposed for the permeability can be utilized for composite manufacturing, e.g., resin transfer moulding processes, and also for validation of advanced models for particle-fluid interactions in a multi-scale coarse grained approach. The improvement/extension of the model for the case of different fiber shape and orientation in 3D for both creeping and inertial flow is left to be carried out in future studies.

ACKNOWLEDGEMENTS

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CALIBRATION OF PARTICLE-BASED MODELS USING CELLS WITH PERIODIC BOUNDARY CONDITIONS

JAN STRÁNSKÝ*, MILAN JIRÁSEK†

* Czech Technical University in Prague
  Faculty of Civil Engineering
  Department of Mechanics
  Thákurova 7, 166 29 Prague 6, Czech Republic
  e-mail: Jan.Stransky.1@fsv.cvut.cz

† Czech Technical University in Prague
  Faculty of Civil Engineering
  Department of Mechanics
  Thákurova 7, 166 29 Prague 6, Czech Republic
  e-mail: Milan.Jirasek@fsv.cvut.cz

Key words: Particle models, calibration, periodic boundary conditions, multi-axial loading, failure envelope

Abstract.

In this contribution, a systematic approach to the calibration of particle models, i.e. characterizing a relationship between microscopic (defined on the level of individual inter-particle bonds) and macroscopic parameters is presented. The procedure is based on simulations of basic cells with periodic boundary conditions (PBC). Firstly, a calibration for elastic properties is explained. A very good agreement between the results of static FEM simulations, quasi-static DEM simulations and theoretical formulas motivated by the microplane theory is found.

Then, basic ideas of calibration of inelastic parameters using PBC are explained on the simple case of uniaxial tension. The dependence of the results on the periodic cell orientation with respect to the localized process zone (that typically occurs in the post-peak range) is studied and the influence of the particle and cell size is covered as well. The gained knowledge is then applied in simulations of material failure under uniaxial compression and multiaxial loading. To demonstrate the applicability of the described method, the plane stress failure envelope for the investigated model is constructed for different combinations of microscopic parameters.
1 INTRODUCTION

Particle-based (or discrete) methods (for example the discrete element method - DEM) are modern tools for numerical simulations, which can be used across many engineering and scientific branches and often beat the most widely used numerical approach – the finite element method (FEM). The discrete methods were originally developed for soil mechanics [1], but nowadays their applications cover structural mechanics [2], fracture analyses [3], impact analyses [4] etc.

In DEM, the studied problem is discretized by discrete elements (e.g. particles), which are mutually connected by deformable bonds. “Microscopic” constitutive parameters of these bonds (e.g. stiffness, strength etc.) influence the behavior of the whole model on the macroscopic scale and the choice of a proper constitutive law and of values of micro-parameters play the key role in the resulting model quality. The micro-parameters are usually identified (calibrated) using some kind of optimization (from the easiest trial-and-error method to sophisticated sensitivity analysis [5]) such that the macroscopic behavior of the model corresponds to the actual behavior (e.g. to the experimentally observed one) as closely as possible.

The topic of DEM calibration was studied by many authors [5, 6, 7, 8], but only a few of them used periodic boundary conditions [9] and, according to our knowledge, there is no study of PBC in combination with post-peak behavior and strain localization. Results of elastic homogenization with PBC lie between bounds evaluated from kinematic and static boundary conditions. In inelastic calibration, using PBC can reduce (unreal) local stress concentrations when applying prescribed displacement or force on certain particles.

In section 2 the chosen particle model is described. Note that the proposed calibration method is applicable to any kind of discrete model. The PBC in context of both DEM and FEM are presented in section 3. Section 4 describes calibration of elastic and inelastic parameters. The effect of mutual orientation of load and periodic cell (causing the direction of strain localization zone in post-peak range) is demonstrated on a simple case of uniaxial tension and observed facts are used and verified on other loading cases. The results are presented in section 5. To demonstrate the applicability of the described method, the plane stress failure envelope for the investigated model is constructed for different combinations of microscopic parameters.

For DEM simulation we used the open-source software YADE [10] and for FEM simulation the open-source software OOFEM [11].

2 INVESTIGATED PARTICLE MODEL

The model used for calibration in this contribution consists of rigid spherical particles with uniform radius $r$. The initial spheres packing is random close created in YADE with dynamic compaction followed by relaxation. Figure 1 shows a very good quality of such packings in terms of packing fraction and bond direction distribution.

Initially, particles whose center distance $l$ is less than $2rI_r$ (where $I_r$ is the so-called
interaction ratio) are connected. Each particle has 6 degrees of freedom (DOFs) – three displacements and three rotations. Each bond is characterized by its length \( l \), unit normal vector \( \mathbf{n} \), cross-section area \( A = \pi r^2 \) and internal forces \( \mathbf{f} \).

Bonds in our model have normal and shear (or transversal) elastic fictitious material stiffness \( E_b \) and \( G_b \) [Pa] and normal and shear bond stiffness \( k_N = E_b A/l \) and \( k_T = G_b A/l \) [N/m] (see fig. 2). In tension we used a bilinear damage mechanics law and in shear a Mohr-Coulomb-like plastic model (see fig. 3). Our simple model has 6 parameters that need to be calibrated, see table 1.

3 PERIODIC BOUNDARY CONDITIONS

Consider a periodic cell as a block filled with a periodic assembly of particles and bonds. Periodicity means that this cell (as well as all its particles and bonds and all their properties – velocity, stress, damage etc.) is surrounded by identical cells shifted along the cell edges, see fig. 4. For both studied methods (static FEM and dynamic DEM) there are special procedures how to incorporate PBC.
Table 1: Model parameters.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_b$</td>
<td>Bond fictitious material normal stiffness</td>
<td>Pa</td>
</tr>
<tr>
<td>$G_b$</td>
<td>Bond fictitious material shear stiffness</td>
<td>Pa</td>
</tr>
<tr>
<td>$\varepsilon_0$</td>
<td>Limit elastic tensile strain</td>
<td>-</td>
</tr>
<tr>
<td>$\varepsilon_f$</td>
<td>Tensile strain when the bond is fully broken</td>
<td>-</td>
</tr>
<tr>
<td>$c_0$</td>
<td>Initial shear bond cohesion</td>
<td>Pa</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>Bond internal friction angle</td>
<td>rad</td>
</tr>
</tbody>
</table>

Figure 3: Considered constitutive law.

3.1 Static FEM solution

The linear part of the described model (including PBC) has been implemented into OOFEM with special nodes representing particles and special finite elements representing bonds. Each particle $P$ has a displacement vector $u_P$. Merging the displacement vectors of connected particles, a bond (element) displacement vector $u$ is constructed and the element strain $\varepsilon$ can be computed as

$$\varepsilon = Bu,$$

where $B$ is element geometric (strain-displacement) matrix. In general, the element stiffness matrix $K^e$ is defined in terms of $B$ and material stiffness matrix $D$ as

$$K^e = \frac{1}{l}B^TDB.$$

The global stiffness matrix is assembled from particular stiffness matrices of all elements. The implementation of the PBC is analogous to [3]. Consider an element connecting one particle inside the cell with another particle physically located in one of the neighboring cells ($J'K$ and its periodic image $JK'$ in fig. 4). PBC are imposed by the set of constraint equations that contain the components of macroscopic deformation $E = \{E_x, E_y, E_z, E_{yz}, E_{zx}, E_{xy}\}^T$. For instance, for link $JK'$ and for $x$ components we write

$$u_{K'} = u_K + E_xk_xC + E_{xy}k_yC, \quad \phi_{xK'} = \phi_{xK}.$$  

$C$ is the dimension of the cubic periodic cell, constants $k$ have values -1, 0 or 1 and specify the position of the particle outside the cell according to the relation (again only
for \( x \) direction)
\[
  x_{K'} = x_K + k_xC.
\]

Using equations (3) and (4), the displacement of connected particles \( K \) and \( J' \) (periodic image of particle \( J \)) can be written in terms of the displacements of particles \( J \) and \( K \) and the macro-deformation \( \mathbf{E} \) as
\[
  \begin{pmatrix}
    u_K \\
    u_{J'}
  \end{pmatrix}
  =
  \mathbf{P}
  \begin{pmatrix}
    u_K \\
    u_J \\
    \mathbf{E}
  \end{pmatrix}.
\]

Using the periodic transformation matrix \( \mathbf{P} \), the modified stiffness matrix of the “periodic” elements can be expressed in the form
\[
  \mathbf{K}^e = \frac{1}{l} \mathbf{P}^T \mathbf{B}^T \mathbf{D} \mathbf{B} \mathbf{P}.
\]

The components of macro-deformation \( \mathbf{E} \) are therefore considered as global degrees of freedom. The corresponding “load” components are directly related to the macro-stress (they are equal to the stress components multiplied by the volume of the cell). To prevent displacement of the assembly as a rigid body, one particle needs to be “supported” by setting its three displacements to zero.

### 3.2 Dynamic DEM solution

The PBC for DEM are implemented in YADE. The periodic simulation is governed by the shape of periodic cell. We can modify the periodic cell via its 3x3 transformation matrix \( \mathbf{T} \) (identity matrix initially) in two basic ways: rotation (when no strain occurs) and deformation (normal or shear strain without rotation), see fig. 4. At the beginning of our simulation, the cell is rotated to the requested position. The computational procedure
in a generic $k$-th step of simulation is as follows: First, the polar decomposition [12]

$$T_k = UH \quad (7)$$

is performed on $T$. $U$ is an orthogonal matrix and $H$ is a positive semi-definite symmetric matrix. Apart from this mathematical definition, polar decomposition has a straightforward geometric meaning: $U$ represents rigid body rotation and $H$ is related to the shape change. In terms of infinitesimal strain theory, the strain $E$ is obtained as

$$E = T - I, \quad (8)$$

where $I$ is the identity matrix. Another definition of strain (e.g. logarithmic) could be incorporated.

The prescribed strain increment (in global coordinates) $\Delta E$ is then appropriately rotated to cell’s local coordinates and added to the shape matrix $H$. Afterwards, the new value of $T$ is composed from $U$ and new $H$:

$$T_k = UH, \quad T_{k+1} = U(H + U^T \Delta EU) \quad (9)$$

Prescribed strain components can be directly applied via the cell’s shape change. However, stress cannot be prescribed directly. Therefore, we developed a special strain predictor, which considers the values of stress and strain in a few last steps and predicts the strain value for the next step such that the value of stress is as close as possible to the prescribed one, see [10] for more details. The stress is computed according to [13] as

$$\sigma = \frac{1}{V} \sum_{b \in V} l \left[ Nf_N + T^T \cdot f_T \right], \quad N = n \otimes n, \quad T^T = I_{sym} \cdot n \otimes n \otimes n$$

$$T^T \cdot f_T = I_{sym} : (n \otimes f_T) - n \otimes n \otimes n \cdot f_T^T$$

$$\sigma = \frac{1}{V} \sum_{b \in V} l \left[ f_N n \otimes n + \frac{1}{2} (n \otimes f_T + f_T \otimes n) \right] \quad (10)$$

$V$ is the cell volume, $n$ is the bond unit normal vector, $f_N$ and $f_T$ are the normal and shear internal forces ($n$ and $f_T$ are perpendicular, therefore $n \cdot f_T = 0$), $N$ and $T$ are projection tensors and $I_{sym}$ is the fourth-order symmetric unit tensor. The sum is performed over all bonds $b$ of the cell.

4 CALIBRATION

4.1 Elastic parameters

To obtain elastic macro-parameters numerically, from the structural response to a prescribed boundary displacement (under this constraint the elastic potential energy is not minimal and the response is stiffer than the real one) or to a prescribed boundary
force load (under this constraint the complementary elastic energy is not minimal and the response is softer than the real one), we can estimate the upper and lower stiffness bounds, respectively. PBC are a compromise between these two bounds and in general leads to better results [9].

A column of the macroscopic elastic stiffness (or compliance) matrix is equal to the macroscopic stress (or strain) caused by macroscopic strain (or stress) with unit value of investigated component and zero values of all other components. This method was used for both FEM and DEM simulations.

Theoretical analytical solution presented in [13] derived from prescribed macroscopic uniform deformation yields an upper bound estimation of elastic stiffness tensor

$$D = \frac{1}{V} \sum_{b \in V} AL \left( E_b \mathbf{N} \otimes \mathbf{N} + G_b \mathbf{T}^T \cdot \mathbf{T} \right)$$

$$D_{ijkl} = \frac{1}{V} \sum_{b \in V} AL \left[ (E_b - G_b) n_i n_j n_k n_l + \frac{1}{4} \left( n_i n_j \delta_{jk} + n_i n_k \delta_{jl} + n_j n_l \delta_{ik} + n_j n_k \delta_{il} \right) \right]$$

Under the assumption of uniform probability of bond direction distribution, the following estimates of elastic constants (Young’s modulus $E$ and Poisson’s ratio $\nu$) can be derived (see [13] for more details):

$$E = E_b \frac{\sum_{b \in V} AL}{V} \frac{2 + 3 \frac{G_b}{E_b}}{4 + \frac{G_b}{E_b}}, \quad \nu = \frac{E_b - G_b}{4E_b + G_b}$$

4.2 Inelastic parameters

PBC are also useful for calibration of inelastic parameters, usually ultimate stress/strain and shape of stress-strain (or force-displacement) diagram under specific load conditions (typically uniaxial tension or compression). For the case of uniaxial tension, a problem can arise when applying prescribed stress/strain on opposite “faces” of a specimen. If the sphere packing of the face is regular, the transition of regular to irregular (random) particle structure is usually broken and damaged first, before the “real structure” can be investigated. Another possibility would be to cut a plane from random packing and fix some particles up to a given distance from the face, but this can lead to stress concentration at the transition of fixed and unfixed particles and devaluation of simulation results. For this reason, the periodic boundary conditions seem to be suitable solution.

However, all that glitters is not gold. In the calibration with the help of PBC, we have to pay attention to the cell orientation with respect to the load, especially if strain localization occurs. In general, there exists an “optimal” orientation of the periodic cell, where the localized zone is parallel to the cell surface or is crossing the cell from one corner to another. For the simple case of uniaxial tension, the optimal orientation is zero. Then the localization zone (crack) has the minimal area (and is only one) and the minimal amount of energy is needed to split the cell. For other orientations, the periodic boundary
conditions force the crack crossing the cell boundary to continue at the periodic image of the cross point on another cell edge (see fig. 5). The crack is then longer than in the ideal case, more energy is needed for its propagation and the behavior of the cell is more ductile (see fig. 8). Notice the same behavior in pre-peak (elastic) range and different behaviors in post-peak (inelastic) range. The most ductile response is exhibited by a cell rotated by about 30°, the most fragile (as expected) by an unrotated cell. Results for 45° lie in between, see fig. 5 for illustrative example.

Figure 5: Different localization zone using PBC for uniaxial tension in horizontal direction

In a general calibration procedure, the most brittle (optimal) cell position has to be found numerically and its behavior is considered as the real one (unaffected by periodic boundary conditions).

5 RESULTS

The results of elastic calibration are summarized in figures 6 and 7, showing numerical and analytical values of Young’s modulus $E$ and Poisson’s ratio $\nu$ for different interaction ratios. The numerical results of static FEM and quasi-static DEM simulations are indistinguishable from each other. The same fact can be observed for the analytical solution according to equations (11) and (13). For higher interaction ratios, the agreement between analytical and numerical solution is better and the analytical solution was verified to be the upper stiffness bound.

The elastic numerical simulations also verified that for a sufficient number of particles the model with random close packing is macroscopically isotropic and the results are rotationally invariant (the deviations get smaller for a higher number of used particles). The elastic results are size-independent.

For the inelastic part of calibration, we firstly verified our strain predictor, then the “quasi-staticity” of simulations and finally the post-peak results dependency on the cell orientation, see fig. 8. For the case of uniaxial tension, the most brittle (“optimal”) behavior is obtained for a non-rotated cell.

Since the model exhibits strain localization, we can expect size effect phenomena. Similarly to pathological mesh size dependence in FEM, when the cell is cracked, the strain is localized into one layer of “elements” (bonds), while the rest of the cell is being unloaded. For a larger cell, the width of the localized area is relatively smaller and
the resulting post-peak behavior is more brittle. This is shown in fig. 9 (almost no influence of the cell size on the elastic branch of the diagram and on the strength, but a significant influence on the post-peak behavior). Thus the microscopic parameters should be calibrated with respect to both particle \((r)\) and cell \((C)\) size. As seen in fig. 9, the results are influenced by the relative size of particles with respect to the cell size rather than by the absolute particle size.

For the case of uniaxial compression, the most fragile behavior occurs approximately for a rotation between \(20^\circ\) and \(30^\circ\) and for simple shear near \(45^\circ\).

An important fact for all the studied cases is that the pre-peak (elastic) response is the same for all orientations (verifying isotropy of the model) and the strength (maximum reached stress) is also almost identical for all cases. Under this assumption, the plane stress failure envelope is constructed for different material parameters in fig. 10.

**Figure 6**: Ratio of macroscopic and bond Young’s moduli \(E/E_b\) as a function of \(G_b/E_b\) ratio.

**Figure 7**: Poisson’s ratio \(\nu\) as a function of \(G_b/E_b\) ratio.
Figure 8: Verification of strain predictor (a), “quasi-staticity” (results are for constant final strain and different number of time steps) (b) and results dependency on cell orientation under uniaxial tension (c).

Figure 9: Results for uniaxial tension with different particle and cell sizes (a), uniaxial compression (b) and simple shear (c).

6 CONCLUSION

A systematic calibration method for discrete models with the help of periodic boundary conditions was presented. This method is applicable to any type of particle model and for both elastic and inelastic material parameters identification. The periodic boundary conditions have a positive influence on the results in the elastic range (it is a compromise between kinematic and static conditions).

In the case of inelastic calibration, PBC can reduce local stresses due to force or displacement prescribed on certain particles. A special attention has to be paid to the cell orientation with respect to the load. For realistic results, the optimal orientation (without negative effects of PBC) has to be found and the parameters should be calibrated on such an orientation. This orientation is parameter-dependent, so by changing the parameters to be optimized, the optimal calibration orientation can be changed as well.
Figure 10: Figures of plane stress failure envelopes for different material parameters.

7 ACKNOWLEDGEMENT

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REFERENCES


DEM SIMULATIONS OF SOIL-PILE INTERFACE UNDER STATIC AND CYCLIC LOADING

RAVI PATEL*, MARTIN ACHMUS†, BALESHWAR SINGH* AND KHALID ABDEL-RAHMAN †

* Civil Engineering Department
Indian Institute of Technology Guwahati
Assam, India.
email: a.patel@iitg.ac.in, webpage: www.iitg.ac.in

† Inst. for Geotechnical Engineering
Leibniz University of Hannover,
Hannover, Germany.
email: achmus@igth.uni-hannover.de, webpage: www.igth.uni-hannover.de

Key words: DEM, soil-pile interface, CNL and CNS tests, static and cyclic loading

ABSTRACT: In this study, Discrete Element Method (DEM) was used to simulate interface direct shear tests for both constant normal load (CNL) and constant normal stiffness (CNS) conditions. The model was calibrated and validated using laboratory data. Simulations were made for both static and cyclic tests for different amplitudes at normal stress levels ranging from 100kPa to 400kPa on sand having relative density of 50%. No major difference was observed between static CNS and CNL tests for shear stress behaviour. However, a decrease in normal stress was observed in CNS tests which were evident from the imposed boundary conditions. In cyclic CNS tests, degradation of shear stress was observed for higher displacement amplitudes. Shear band thickness was measured from rotation diagrams and was observed to be 5 to 10 times $D_{50}$ for all the tests.

1 INTRODUCTION

Direct shear apparatus is often used in the laboratory to study soil-pile interface behaviour. The normal load boundary condition employed in direct shear apparatus can be expressed as follows:

$$\sigma_n = \sigma_{n0} - K \Delta z$$  \hspace{1cm} (1)

where, $\sigma_n$ is the current normal stress level, $\sigma_{n0}$ is the initial normal stress level, $K$ is the spring stiffness and $\Delta z$ is the deformation of the specimen normal to the interface.

Three different kinds of normal stress boundary conditions can be employed in direct shear tests:

1. **Constant normal load test (CNL test):** The normal load is constant ($K=0$, $\Delta z \neq 0$, $d\sigma_n = 0$) similar to drained condition. In this case the interface may compress or dilate freely.
2. **Constant volume test (CV test):** The volume of soil remains constant \((K = \infty, \Delta z = 0, \ \delta \sigma_n \neq 0)\) similar to undrained condition. During this test as no displacement of upper boundary wall is allowed, the normal stress may increase or decrease depending on the tendency of soil to dilate or contract.

3. **Constant normal stiffness test (CNS test):** The normal load is adjusted by a spring constant to replicate the degradation of normal stress from far field soil \((K=\text{constant}, \Delta z \neq 0, \delta \sigma_n \neq 0)\).

   CNL represents lower bound case where as CV represents upper bound case of CNS test. It has been well established that the pile-soil interface behaviour can be investigated using CNS direct shear tests. Experimental studies have been reported by different researchers on the influence of factors such as initial normal stress, spring stiffness, soil type, relative density, interface surface roughness and magnitude of loading in CNS direct shear apparatus on global specimen response [1−4]. A micro-scale investigation of CNS test results conducted on sand in transparent sided apparatus using PIV analysis showed that the degradation of normal stress in CNS test is due to the contraction and rearrangement of particles occurring in narrow shear band [5]. The aim of this paper is to develop a DEM model to simulate direct shear interface tests and to understand the behaviour of sand-pile interface using these simulations for both static and cyclic tests.

### 2 SIMULATION PROCEDURE

Two dimensional DEM simulations were carried out using DEM code *PFC*\(^{2D}\) [6]. In *PFC*\(^{2D}\), sand particles are modelled as disks of unit thickness and the boundaries are modelled by walls. The interaction between disks (or disk and wall) is determined using contact laws. A typical calculation cycle in *PFC*\(^{2D}\) consists of determining forces on disks based on their relative positions using contact laws and updating the position of disk by integration of Newton’s second law of motion.

![Grain size distribution curve of modelled sand](image-url)
For simulations, linear elastic contact law with Coulomb friction was employed with local damping (damping ratio 0.7) to dissipate the excess kinetic energy. Sand modelled was poorly graded quartz sand (Uniformity index $U = 2.2$; index of curvature $C_c = 1.0$ and mean particle diameter $D_{50} = 0.42\text{mm}$) with grain size distribution as shown in Fig. 1. The dimensions of the interface shear apparatus used in the laboratory was 300 x 300 x 50mm but for simulations, size employed was 180 x 30mm to reduce number of particles and computation time.

Simulation was carried out in three phases:

Phase 1: Side walls and bottom wall with teeth (which represents interface roughness) were constructed. Particles were generated with required grain size distribution by dividing grain size distribution curve in five parts, and were allowed to settle under gravity until equilibrium was achieved. The relative density of generated specimen was found using the following relation [7]:

$$R_d = \frac{0.214 - \eta_{2D}}{0.214 - 0.141} \quad (2)$$

where, $R_d$ is the relative density of the sample and $\eta_{2D}$ is the porosity achieved at the end of phase 1, 0.214 corresponds to maximum porosity than can be attained at the end of phase 1 for inter-particle coulomb friction coefficient equal to 25 and 0.141 corresponds to the minimum porosity that can be attained at the end of phase 1 for inter-particle coulomb friction coefficient equal to 0.

Phase 2: The top wall is constructed and initial stress conditions are set using servo controlled mechanism.

Phase 3: In this phase, shearing of the sample is carried out. The boundary conditions are maintained as given by equation (1) using servo control mechanism. Fig. 2 shows the schematic diagram of the developed model of CNS test in $PFC^{2D}$ code.

![Schematic diagram of CNS test in $PFC^{2D}$](image)

**Fig. 2.** Schematic diagram of CNS test in $PFC^{2D}$
3 CALIBRATION

The model was calibrated and validated under both CNL and CNS conditions using appropriate dimensions of interface teeth which approximate roughness of the surface and adjusting appropriate contact law parameters. To set guidelines for calibration, initial simulations were made to understand the influence of teeth parameters and contact law parameters on CNL test.

Increase in tooth height or increase in slope angle (angle made by inclination of tooth with horizontal) causes increase in interface coefficient of friction. Higher slope angle causes high undulations on shear stress-displacement curves due to frequent loss of contact between wall and particles and hence the slope angle should not be kept higher than 30°.

![Graph showing the relationship between coulomb coefficient of friction and peak interface coefficient of friction](image)

**Fig. 3.** Relationship between coulomb coefficient of friction and peak interface coefficient of friction

To understand influence of contact parameters for linear elastic contact law viz., normal contact stiffness ($K_n$), shear contact stiffness ($k_s$) and inter-particle coulomb friction coefficient ($\mu_e$), simulations were carried out by changing one parameter at a time and keeping the other parameters as constant. It was observed that the increase in $\mu_e$ caused increase in peak shear stress while keeping shear modulus and residual shear stress constant. The relation between the inter-particle coulomb friction coefficient ($\mu_e$) and peak interface friction coefficient ($\mu_{peak}$) is shown in Fig. 3. Increase in $K_n$ led to increase in the shear modulus, peak stress values and residual stress values. Change in value of $k_s$ had no influence on shear stress displacement behaviour. Higher $\mu_e$, $K_n$, and $k_s$ values showed dilatant behaviour in contrast to the contractive behaviour observed for lower values.

The final values of parameters adapted for calibrated model are as shown in Table 1. The model was calibrated and validated with laboratory CNS test data reported for the same sand with 50% relative density [8]. Comparison between results from developed DEM model and experiments are shown in Fig. 4. Comparisons were made for initial normal stress of 100, 200, 300, and 400kPa with spring constants of 48, 120, 96, and 120kPa/mm, respectively.
Good agreement was observed between experimental results and DEM model results for both shear stress and change in normal stress. The results of calibrated model matched consistently at all stress levels.

**Table 1. Parameters for calibrated model**

<table>
<thead>
<tr>
<th>Entity</th>
<th>Properties</th>
</tr>
</thead>
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<tr>
<td><strong>Balls</strong></td>
<td>Density ($\rho = 2649$ kg/m$^3$)</td>
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<tr>
<td></td>
<td>Normal contact stiffness ($K_n = 4 \times 10^6$ N/m)</td>
</tr>
<tr>
<td></td>
<td>Shear contact stiffness ($K_s = 2 \times 10^6$ N/m)</td>
</tr>
<tr>
<td></td>
<td>Inter particle friction coefficient ($\mu_e = 0.17$)</td>
</tr>
<tr>
<td><strong>Walls</strong></td>
<td>Normal contact stiffness ($K_n = 1 \times 10^9$ N/m)</td>
</tr>
<tr>
<td></td>
<td>Shear contact stiffness ($K_s = 0$ N/m)</td>
</tr>
<tr>
<td></td>
<td>Friction coefficient ($\mu_e = 0$)</td>
</tr>
<tr>
<td><strong>Interface teeth</strong></td>
<td>Height of teeth = 1.26mm ($3 \times D_{50}$)</td>
</tr>
<tr>
<td></td>
<td>Angle of inclination of teeth with horizontal = 30°</td>
</tr>
</tbody>
</table>

![Graph showing comparison between the Calibrated DEM model and laboratory CNS test results](image)

**Fig. 4.** Comparison between the Calibrated DEM model and laboratory CNS test results

4 RESULTS

Static CNL and static and cyclic CNS tests were carried out for normal stress levels of 100, 200, 300 and 400kPa with spring stiffness values of 88, 184, 288 and 368kPa/mm, respectively. Higher values of K are taken for higher stress level as K is directly proportional to far field small strain shear stiffness [9] in case of pile foundations and this small strain stiffness is found to increase with stress level [10]. All tests were carried out on sand sample with relative density 50% (medium dense sand).
Results of CNL test are shown in Fig. 5. Contractive behaviour was observed for CNL test and the coefficient of interface friction was found to be 0.233. Figure 6 shows the comparison between static CNL and CNS tests for normal load level of 100kPa, and similar behaviour was observed for other stress levels. No major change in shear stress displacement behaviour was observed but the decrease in normal stress was evident due to imposed CNS condition.

Cyclic CNS test simulations were carried out to understand the influence of displacement amplitude. Figure 7 shows degradation factors for maximum shear stress at different stress levels and different displacement amplitudes. Degradation factor is defined as the ratio of soil property under cyclic loading to that under static loading. It was observed for all stress levels that lower displacements (0 to 0.5mm and 0 to 1mm) had less effect on shear stress capacity of the soil, whereas higher displacements (0 to 2mm and 0 to 5mm) resulted in degradation in shear capacity of soil by about 20%. Similar behaviour for different displacement amplitudes has been reported in experimental studies by different researchers [2, 4, 11].
Fig. 7. Degradation factor for cyclic CNS tests with different displacement amplitudes

Fig. 8. Development of rotations in cyclic CNS tests. ($\sigma_{\text{min}} = 100\text{kPa}, K = 88\text{ kPa/mm}, \text{Displacement} = 0\text{-}2\text{mm}$)
Rotations of particles can give clear indication of shear band formation [12]. As shearing progresses, higher rotation of the particles is observed near interface due to particle agitation and rearrangement in both static and cyclic tests. Distinct shear band could be observed in the rotation diagrams. Figure 8 shows development of shear band as cycling progresses. The shear band thickness was found to be dependent on displacement amplitude for cyclic loading. Larger shear band thickness was observed for higher displacement amplitudes. The shear band thickness at the end of all tests for both static and cyclic CNS tests was found to be varying from 5 to 10 times of $D_{50}$.

5 CONCLUSIONS

DEM simulations were able to reproduce the behaviour of interface direct shear test under different boundary conditions.

Increase in teeth height or teeth slope angle resulted in increase in interface friction. Teeth slope angle should not be greater than 30° for smooth stress displacement curves. Higher inter-particle coulomb friction coefficient resulted in higher peak stresses. $K_n$ affects the overall behaviour of the sample and should be carefully chosen. Larger shear modulus peak stress and residual stresses where observed for higher $K_n$ value. $k_s$ has no effect on stress displacement behaviour. Higher $K_n$, $k_s$ and inter-particle coulomb friction coefficient resulted in dilatant behaviour in contrast to contractive behaviour for lower values. These points serve as guidelines for calibrating interface direct shear test DEM models.

No major difference was observed between static CNS and CNL tests for shear stress behaviour on sample with relative density of 50%. However, a decrease in normal stress was observed in CNS tests which were evident from the imposed boundary conditions. In cyclic CNS tests, no degradation was observed for lower displacement amplitudes but higher displacement amplitudes led to degradation of shear capacity by about 20%. Shear band thickness was measured from rotation diagrams and was observed to be 5 to 10 times $D_{50}$ for all the tests. Thicker shear band was observed for higher displacement amplitudes.

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FAILURE IN POROUS GRANULAR AGGREGATES

R. Affes∗+, V. Topin++, J-Y. Delenne+, Y. Monerie++ AND F. Radja++

∗LMGC CNRS-Université Montpellier II, Place Eugène Bataillon, 34095 Montpellier Cedex
++IRSN, DPAM, CE Cadarache, Bat. 702, BP3-13115 St. Paul-lez-Durance Cedex
+,++ Laboratoire MIST, IRSN-CNRS-Université Montpellier II, France

∗ rafik.affes@univ-montp2.fr

Key words: Porous granular aggregates, Lattice model, Fracture, Crack path, Tortuosity

Abstract. We use a 3D Lattice Element Method, based on the discretization of the particles and binding matrix on a regular lattice, to investigate the particle-scale origins of the strength and failure of porous granular aggregates under tensile loading. Damage growth is analyzed by considering the evolution of stress probability density and the number of broken bonds in the particle phase. We show that the stress probability density functions are increasingly broader for a decreasing matrix volume fraction, the stresses being more and more concentrated in the interparticle contact zones with an exponential distribution as in cohesionless granular media [4]. We carried out a detailed parametric study in order to evaluate the combined influence of the matrix volume fraction and particle-matrix adherence. Our findings are in agreement with 2D results previously reported in the literature [6]. Three regimes of crack propagation are evidenced, corresponding to no particle damage, particle abrasion and particle fragmentation, respectively. The crack morphology (tortuosity...) is another important feature that we investigate for different distributions of the particles and pores within porous granular aggregates.

1 Introduction

Dense granular materials are characterized either in terms of the network of solid particles or by the properties of the pore space which can be fully or partially filled by a solid binding matrix or a liquid. At high particle volume fractions $\rho_p$ (typically, for $\rho_p > 0.57$), the stress transmission is basically guided by a percolating network of inter-particle contacts [5]. This role of the contact network in force transmission and rheological behavior has been mainly investigated in granular materials in the absence of a binding matrix and under compressive confining stresses [2, 4].
The issue of stress concentration and the role of particles are much less evident in the presence of a binding matrix and under tensile loading. Such porous granular aggregates have been recently studied in some detail in a 2D geometry by means of numerical simulations [1, 6]. The overall stiffness and tensile strength of these materials are dependent on the matrix volume fraction $\rho_m$, particle volume fraction $\rho_p$ and particle-matrix adhesion $\sigma_{pm}$.

In this paper, we introduce the lattice element method (LEM) in a 3D geometry for the simulation of porous granular aggregates of spherical particles with a solid matrix. Based on a lattice discretization of both phases and their interface as well as an efficient quasi-static time-stepping scheme, the LEM algorithm allows us to analyze the fracture of cohesive aggregates as a function of phase volume fractions and local binding strength.

2 Lattice Element Method

The lattice element method (LEM) has been recently employed as an alternative to the finite element method for the investigation of the fracture properties of granular materials mixed with a binding matrix [1, 6]. Such materials, to which we refer in this paper as porous granular aggregates or cemented granular materials can be found in very different forms in nature and industry. Well-known examples are conglomerates and concrete.

In LEM, the space is discretized as a regular or disordered grid of points (nodes) interconnected by one-dimensional elements (bonds). Each bond can transfer normal force, shear force and bending moment up to a threshold in force or energy. Various rheological behaviors can be carried by these material lattice bonds, in contrast to the finite element approach where the local behavior is carried by volume elements. When several phases are present as in a porous granular aggregates, each phase and its boundaries are materialized by lattice elements sharing the same properties and belonging to the same portion of space. We use linear elastic-brittle elements, each element characterized by a Hooke constant and a breaking force threshold. The bonds transmit only normal forces between the lattice nodes and thus the strength of the lattice in shear and distortion is ensured only by the high connectivity of the nodes. This simple kinematics allows to investigate high sampling statistical approach. A sample is defined by its contour and the configuration of the phases in space. The samples are deformed by imposing displacements or forces to nodes belonging to the contour. The initial state is the reference (unstressed) configuration. The total elastic energy of the system is a convex function of node displacements and thus finding the unique equilibrium configuration of the nodes amounts to a minimization problem (implemented here by means of the conjugate gradient method). Performing this minimization for stepwise loading corresponds to subjecting the system to a quasi-static deformation process. The overloaded elements (exceeding a threshold) are removed according to a breaking rule. This corresponds to irreversible micro-cracking of the lattice. The released elastic energy between two successive equilibrium states is thus fully dissipated by micro-cracking. In the fast implementation used in the present work, all overloaded elements occurring within the same step are removed, as well as those
appearing recursively after energy minimization (within the same step). This corresponds physically to unstable growth of the micro-cracks compared to the imposed strain rate.

The 3D LEM has the advantage to be cheap in computational effort, making it possible to simulate systems with an large number of nodes for reasonable computing time. It should be remarked that due to the simple additivity of the potential energy, the computation time depends only linearly on the number of nodes. It is also obvious that the LEM is a convenient model of brittle fracture in which the generation and propagation of cracks are “naturally” taken into account.

3 Application to granular aggregates

In a granular aggregate, there are three bulk phases: particles, matrix and voids. There are also two interface phases: particle-particle and particle-matrix; see Fig. 1. To construct the samples, we first generate a large dense packing of rigid spherical particles compressed isotropically by means of the contact dynamics method. A cubic portion of this three-dimensional packing is overlaid on a disordered tetrahedral lattice. The particle properties are attributed to the bonds falling in the bulk of the particle phase. The binding matrix is then added in the form of bridges of variable width connecting neighboring particles within a prescribed gap between particles. The bonds belonging to these bridges are given the properties of the matrix. In the same way, the bonds falling between a particle and the matrix or between two particles are given the properties of the corresponding interface. The width of solid bridges between particles is proportional to the total volume of the binding material. At higher levels of the matrix volume fraction, the bridges overlap and the porosity declines to zero. The particles are polydisperse with
diameters varying nearly uniformly in size in a range \([0.8d, d]\). The total particle volume fraction is about 0.6 corresponding to a dense close packing. The samples consist of the bulk phases: 1) particles, denoted \(p\); 2) matrix, denoted \(m\); and 3) void space or pores, denoted \(v\), as well as the interface phases: 1) particle-particle interface, denoted \(pp\), and 2) particle-matrix interface, denoted \(pm\). The elements belonging to each phase \(\phi\) (bulk or interface) are given a Hooke constant \(k^\phi\) and a breaking force \(f^\phi\). We have \(f^v = 0\) and the choice of the value of \(k^v\) is immaterial. The interface phases \(pm\) and \(pp\) are transition zones of finite width. But for large systems, the volume fractions of these transition zones are negligible compared to those of the particles and matrix. The interface phases affect the global behavior through their specific surface and their strengths represented by the Hooke constants \(k^{pp}\) and \(k^{pm}\) and the corresponding tensile force thresholds \(f^{pp}\) and \(f^{pm}\).

In our simulations, we model the interface phases by a one bond-thick layer linking two particles or a particle to the matrix. The volume fractions of the interface phases are thus assumed to be zero \((\rho^{pp} = \rho^{pm} = 0)\) and the volume fractions \(\rho^p\), \(\rho^m\) and \(\rho^v\) are attributed only to the three bulk phases, with \(\rho^p + \rho^m + \rho^v = 1\). It is dimensionally convenient to express the bond characteristics in stress units. We thus define the bond breaking (or debonding) stresses \(\sigma^\phi = \frac{f^\phi}{a}\) and the moduli \(E^\phi = \frac{k^\phi}{a^2}\) where \(a\) is the length of the lattice vector. These bond moduli \(E^\phi\) of the lattice should be carefully distinguished from the equivalent phase moduli which depend both on the bond moduli and the geometry of the lattice. We will use below square brackets to represent the phase moduli: \(E^{[p]}\), \(E^{[m]}\), \(E^{[pp]}\) and \(E^{[pm]}\). It can be shown that the overall Young modulus and Poisson ratio of an disordered isotropic tetrahedral lattice are \(E^{eff} = \frac{5}{3\sqrt{2}}E^\phi\) and \(\nu^{eff} = 0.25\). We performed a serie of simple tension tests over samples composed of 516 particles. The particle volume fraction was kept constant \(\rho^p = 0.6\), and \(\rho^m\) was varied from \(\rho^m/10\) to \(4\rho^m\). Each sample

Figure 2: Normalized vertical stress as a function of vertical strain in tension for two values of the matrix volume fraction \(\rho^m\) (in %).
was discretized over a lattice containing about $1.5 \times 10^6$ elements. The results presented below were obtained for hard particles $E^p = 3E^m$, $\sigma^p = \sigma^m$ and $\sigma^{pp} = 0$. The cubic samples were subjected to uniaxial tension with free lateral sides. The nodes belonging to the base were constrained to be immobile. Upward step-wise displacements were applied to the nodes belonging to the upper surface.

Fig. 2 shows the stress-strain plot under for $\rho^m = 28\%$ and $\rho^m = 13\%$. We observe a brittle behavior with a well-defined initial stiffness $E_{\text{eff}}$ and a tensile strength $\sigma_{\text{eff}}$ at the stress peak. The post-peak behavior is characterized by nonlinear propagation of the main crack (initiated at the stress peak) in the form of a sequence of loading-unloading events. The stiffness declines due to progressive damage of the aggregate. The overall tensile strength is higher at larger $\rho^m$ as a result of a weaker concentration of stresses.

The probability distribution functions of vertical node stresses $\sigma_{zz}^i$ are shown in Fig. 3. From the shapes of the pdf’s, we distinguish large stresses falling off exponentially as observed for large contact forces in granular media [2, 4]. The weak stresses have nonzero probability (increasing as $\sigma_{zz} \to 0$) reflecting the arching effect whereas intermediate stresses are centered on the mean and define a nearly Gaussian distribution. The large stresses mostly concentrate at the contact zones and they form well-defined chains that cross the particles.

The tensile strength and crack propagation are controlled by both $\rho^m$ and $\sigma^{pm}$. For a quantitative evaluation of this effect, we consider here the proportion $n_b$ of broken bonds inside the particles with respect to the total number of broken bonds. Fig. 4 shows a map of $n_b$ in the parameter space $(\rho^m, \sigma^{pm})$ following failure. We see that below a well-defined frontier, no particle damage occurs ($n_b \simeq 0$). For this range of parameter values, the cracks propagate either in the matrix or at the particle-matrix interface. Above this “particle-
damage” limit, the isovalue lines become nearly parallel to the limit line with an increasing level of $n_b$. This suggests three distinct regimes of crack propagation: 1) below the particle-damage limit, the cracks bypass the particles and propagate through the matrix, the pores or along the particle-matrix interface; 2) above this limit and for $\rho^m < 20$, the cracks penetrate into the particles from solid bridges that strongly concentrate stresses; 3) Above this limit, the cracks propagate inside the matrix as well as across the particles, causing the fragmentation of the particles. These results are qualitatively similar in 2D cohesive granular aggregates [6].

4 TORTUOSITY

In order to understand the role of disorder in granular aggregates on the overall crack path, we investigate the effects of size polydispersity and particle volume fraction on the crack tortuosity. A commonly-used estimate of tortuosity can be obtained as the ratio of the length of the crack path to the distance between its end points. This measure is a dimensionless number greater than 1 and it can be applied to a 2D or 3D crack path Fig.5.

Figure 4: Grey level map of the fraction of broken bonds in the particle phase for different values of matrix volume fraction and particle-matrix adhesion.
We first conducted a parametric study in 2 dimensions on square samples under tensile loading simulated by LEM. The particle volume fraction $\rho_p$ varies from 0.35 to 0.55 and the polydispersity varies with the size ratio $r = d_{max}/d_{min}$ between the largest and smallest particle sizes $d_{max}$ and $d_{min}$ for each configuration of $\rho_p$, from 1 (monodisperse) to 7. In order to get sufficient statistics, five different samples for each set of parameters are generated using a deal-leave process ensuring the control of the particle volume fraction and size polydispersity.

The main elastic parameters of the matrix and the aggregate are those of ordinary concrete. The interface between aggregate and mortar is known to have a remarkable effect on the tensile properties of concrete [3] since it constitutes a preferential locus of the failure. To preserve this property, the stiffness of the aggregate/matrix and the aggregate/aggregate interfaces are assumed to be two times less than that of the matrix.

The LEM simulation provides the evolution of fracture as a sequence of 3D images. A dedicated image processing algorithm was developed to extract the crack path from these images and to analyze its morphological properties Fig.6.
Figure 6: Image processing: (a) extracting the crack from sample, (b) binarized crack, (c) skeletonized crack, (d) extraction of largest shortest path (in red)

The evolution of the tortuosity for a given particle volume fraction and three values of size ratio $r$ is displayed in Fig. 7. The mean tortuosity increases with polydispersity in the samples: since the crack is locally reoriented by the boundaries of the aggregates, the apparent tortuosity obtained in a mono-disperse configuration is reproduced at various scales when the polydispersity increases.
Fig 8 displays two snapshots after the appearance of the cracks for the monodisperse sample (a) and sample with $r=5$ (b). In Fig 8(a) the crack passes through the sample between the particles without being deflected from its trajectory. On the other hand in Fig.8(b), the crack is clearly deviated from its trajectory to reach the large particles, increasing thus the tortuosity.
In a forthcoming work, this result will be confirmed in the three dimensional case, and the connection between microstructure and the overall permeability will be investigated.

5 Conclusion

In this paper, a lattice-based discretization approach (lattice element method) was introduced and illustrated by application to the brittle failure of porous granular aggregates. In contrast to dilute particle-reinforced composites, such materials involve a high level of particle volume fraction and thus a jammed skeleton of solid particles interconnected via a binding matrix. The overall behavior depends on the bulk phase volume fractions and the properties of the particle-particle and particle-matrix interface zones. We found that the presence of the particle skeleton controls stress concentration and thus the strength properties of these materials. It was also shown that for a range of the values of the particle-matrix adhesion and matrix volume fraction, no particle damage occurs. The trends are very similar to those previously established for 2D aggregates by the same model.

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FRACTURING IN CONCRETE VIA LATTICE-PARTICLE MODEL

JAN ELIÁŠ* AND ZDENĚK P. BAŽANT†

* Masaryk-Fulbright Fellow, Northwestern University; Assistant Professor on leave from the Brno University of Technology, Czech Republic. e-mail: elias.j@fce.vutbr.cz

† McCormick School Professor and W.P. Murphy Professor of Civil Engineering and Materials Science, Northwestern University, 2145 Sheridan Rd., CEE, Evanston, Illinois 60208; corresponding author, e-mail: z-bazant@northwestern.edu

Key words: fracture, concrete, lattice-particle model, size effect, notch variability

Abstract. Numerical simulation is used to explore the behavior of concrete beams of different sizes and different notch lengths, loaded in three-point bending. The entire range of notch depth is studied. One limit case is type 1 fracture, which occurs when the notch depth is zero and the crack initiates from a smooth surface (this is the case of the modulus of rupture test). Another limit is type 2 fracture, which occurs for deep enough notches. Both cases exhibit very different size effects. The fracture is simulated numerically with a robust mesolevel lattice-particle model. The results shed light on the transitional behavior in which the notch depth is non-zero but not deep enough for developing the the type 2 size effect dominated by energy release from the structure. In agreement with experimental observations and theoretical predictions, the numerical results show evidence of a decreasing macroscopic fracture energy as the ligament gets very short.

1 INTRODUCTION

Modeling of the initiation and propagation of cracks in quasibrittle materials exhibiting strain softening has been studied for several decades. Although this is a difficult task complicated by the distributed damage dissipating energy within a fracture process zone (FPZ) of non-negligible size, realistic results have been achieved by some approaches; see e.g. [1]. In this contribution, the fracturing in concrete is modelled by the lattice-particle model developed in [2, 3, 4].

The main goal is to describe the transition between two basic types of failure. In type 1, a macroscopic crack initiates from a smooth surface and, in type 2, the crack
initiates from a sufficiently deep notch or preexisting fatigued (stress-free) crack. Simple laws giving good approximations of test data have been derived for both types. However, the transition between these two types in the case of very shallow notches remains to be a challenge.

In type 1, a large zone of distributed fracturing develops at the smooth surface until the damage localizes into a crack in the statistically weakest place described by the weakest-link model. In type 2, by contrast, the location of the crack is not random and a much smaller zone of distributed damage grows at a fixed place, the notch tip, until a state of critical energy release rate is reached.

As the notch is getting shallower, the size of the damage zone increases and the crack location gradually develops random scatter. However, up to now there exists no experimental evidence for this transition, and so experiments to characterize it are in preparation at Northwestern University. The present purpose is to clarify this transition by numerical simulations, considering geometrically similar three-point bend concrete beams of constant thickness $b$, various depths $D$ and various relative notch depths $\alpha_0$.

The present analysis is based on the cohesive crack model [5, 6, 1] (also called fictitious crack model). In this model, it is assumed that the cohesive stress transmitted across the crack is released gradually as a decreasing function of the crack opening, called the cohesive softening curve. Its main characteristic is the total fracture energy, $G_F$ – a material constant representing the area under this curve. For stationary propagation, the $J$-integral shows that $G_F$ also represents the flux of energy into the FPZ.

The fracture energy dissipation occurs within numerous meso-level microcracks in the FPZ. The present numerical model will directly simulate the behavior of these microcracks on the meso-level of a brittle inhomogeneous material such as concrete. For this purpose, the present analysis will be based on the discrete lattice-particle developed by G. Cusatis and coworkers [4], which is an extension of [2, 3]. The meso-level material fracture properties are in this model characterized by stress-displacement relations at the interfaces between grains or particles, representing the mineral aggregates in concrete.

2 BRIEF MODEL DESCRIPTION

The material is represented as a discrete three-dimensional assembly of rigid cells. The cells are created by tessellation according to pseudo-random locations and radii of computer generated grains/particles. Every cell contains one grain (Fig. 1a,b). On the level of rigid cell connection, the cohesive crack model is used to represent the cracking in the matrix between the adjacent grains. The fracture energy is the same for all connections except that it depends on the direction of straining. The inter-particle fracturing is assumed to be of damage mechanics type. Thus the plastic frictional slip is not separately accounted for. But this simplification would matter only for unloading behavior which is not the objective of the present analysis. For a detailed description of the connection constitutive law or other model features, see [4]. However, the following minor deviations from the model in [4] are introduced:
• The interparticle connection cohesive law in tension and shear is bilinear instead of exponential. It is therefore defined by eight constants: i) initial mesolevel fracture energy in tension and pure shear, $G_t$ and $G_s$; ii) total mesolevel fracture energy in tension and pure shear, $G_T$ and $G_S$; iii) the mesolevel cohesive tensile and shear strengths, $\sigma_t$ and $\sigma_s$, and iv) the coordinates of the "knee point", i.e., the intersection of the two linear segments considered as 20% of tensile strength $\sigma_t$ or shear strength $\sigma_s$, respectively.

• The notch is represented simply by removing all the connections that cross the midspan provided that at least one of the centers of the connected particles is closer to the crack mouth than $\alpha_0 D$. The advantage of this approach is that all grain positions can be completely random, and that the cutting of the notch by a saw is represented faithfully. The disadvantages are that the notch tip location is not exact and it is impossible to introduce notches whose depth is less than the minimal grain radius.

• The confinement effect is neglected, but it was estimated that, in this type of experiment, the confinement does not play any important role.

The mesolevel material properties in this model are deterministic. Randomness is introduced solely by pseudo-random locations and radii of grains. The effect of spatial
variability of the material properties, which was found to be very important for capturing the statistical (Weibull) part of the type 1 size effect [7, 8]), is neglected. Since all the interparticle connections have identical deterministic fracture energy and tensile strength, the crack initiation from a smooth surface is preceded by distributed fracturing along the entire bottom surface. Nevertheless, the localized macroscopic crack always initiates very close to the midspan (Fig. 1e).

3 SIMULATION OF BEAMS OF VARIOUS SIZES AND NOTCH DEPTHS

Beams geometrically similar in two dimensions, having depths $D = 100, 200, 300, 400$ and 500 mm and the same thickness of $t = 0.04$ m, were modelled. The span-depth ratio was $S/D = 2.4$, and the maximal aggregate diameter was 9.5 mm. The minimal grain diameter was chosen as 3 mm. Based on the Fuller curve, particles of radii within chosen range were generated and pseudo-randomly placed into the specimen domain. The parameters of the connection constitutive law, which were mostly taken similar to those in [4], were: $E_c = 30$ GPa; $E_a = 90$ GPa; $\sigma_t = 2.7$ MPa; $G_t = 15$ N/m; $G_T = 30$ N/m; $\sigma_s = 3\sigma_t = 8.1$ MPa; $G_s = 215$ N/m; $G_S = 430$ N/m; $\sigma_c = 16\sigma_t = 43.2$ MPa; $K_c = 7.8$ GPa; $\alpha = 0.15$; $\beta = 1$; $\mu = 0.2$; $n_c = 2$.

To ensure numerical stability in presence of softening, the simulations were controlled by prescribing the increase of the crack mouth opening displacement (CMOD) in every step. For unnotched beams, the location of macrocrack initiation was not known in advance, and so the controlling displacement was chosen to span several maximum aggregate sizes along the tensile face of the beam.

To save computer time, the lattice-particle model covered only the region in which cracking was deemed to be possible. The region in which no damage was expected was assumed to follow linear elasticity and was modelled by standard 8-node isoparametric finite elements. The elastic constants for these elements were identified by fitting a displacement field with homogeneous strain to the discrete field of particle displacements generated at low stress level for a prism of particles subjected to low-level uniaxial compression. The macroscopic Young’s modulus and Poisson ratio were thus found to be $E = 30.3$ GPa and $\nu = 0.225$. The finite element mesh was connected to the system of particles by introducing interface nodes treated as auxiliary zero-diameter particles (Fig. 1d). Same as the standard particles of the lattice model, these auxiliary particles had three translational and three rotational degrees of freedom. Each auxiliary particle lied at the boundary of one finite element. A similar interfacing was used in [3] but here, in contrast, the FEM nodes were considered to be the masters, and the auxiliary particle displacements were dictated by the master displacements according to the master element shape (or interpolation) functions. The rotations of the auxiliary particles were unconstrained.

For large specimens and shallow notches, many particles are needed to fill the damage region. This led to extreme computational time and memory requirements. Therefore, such simulations were terminated as soon as the load dropped to 90% of the peak force.
The benefit was that there was no need to simulate the crack in the upper part of the beam, and thus many fewer particles were needed. For unnotched beams or beams with deep notches, respectively, the simulations were run until the load was reduced to 40% or 5% of the peak load.

Six realizations were computed for unnotched specimens of each size and for relative notch depth $\alpha_0 = a/D = 0.5$, but only three realizations for other notch depths, i.e., for $\alpha_0 \in \{0.01, 0.02, 0.03, 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.7, 0.8, 0.9\}$.

According to a procedure developed in [4], the depth of specimen was divided into horizontal strips of width $h = 12$ mm (Fig. 1c). The average stress $\sigma_x$ normal to the crack plane and the energy $g_d$ dissipated per unit area were measured and stored for each strip and each step. This allowed reconstructing the macroscopic cohesive softening law in postprocessing. The $\sigma_x$ value was obtained as the stress that must be applied on a vertical section through the center of each cell (Fig. 1b) to ensure equilibrium of both parts [9].

4 OBSERVED NOTCHED-UNNOTCHED TRANSITION

The simulations of beams with no notch (type 1) and deep notch (type 2) behaved as expected. A large fracturing zone developed before the peak load in the case of initiation from a smooth surface (type 1) (Fig. 2). For deep notches, the damage was localized above the notch tip only. For shallow notches, the damage above the tip prevailed but some mesolevel cracking along the bottom surface took place as well.

A qualitatively different damage pattern at peak load was obtained comparing the shallowest notch and no notch simulations (Fig. 2 $\alpha_0 = 0$ and 0.01). The smallest size $D = 100$ mm and smallest notch $\alpha_0 = 0.01$ (for which the actual notch depth is only 1 mm) was an exception. The procedure used for notch creation did not lead to the removal of any contact and so no notch was actually introduced. Similarly, a notch of
Figure 3: Sums of energy per unit area dissipated in strips until stress $\sigma_x$ in each strip gets reduced in post-peak to 75% of the tensile strength $\sigma_t$.

the depth of 2 mm (obtained for $D = 100$ mm, $\alpha_0 = 0.02$ and $D = 200$ mm, $\alpha_0 = 0.01$) was represented poorly because only a few contacts, discontinuous through the specimen width, were severed. The simulation with mesolevel refinement of the microstructure does not suffice for capturing the effect of notches smaller than the dominant mesolevel inhomogeneities. A deeper refinement of microstructure simulation would be needed to capture the precise notch tip, but it would considerably complicate the programming.

Based on the observed damage patterns at the peak, the type 1–type 2 transition begins immediately upon introducing any notch exceeding the size of the dominant inhomogeneity (> 3 mm). Considering that the pure type 2 behavior is reached when almost no cracking occurs at the bottom surface, the transition becomes complete when the notch depth is about 10–15 mm (see Fig. 2 for size $D = 300$ mm). This is about 1.5 maximum aggregate size.

The difference between the type 1 and type 2 fracture behaviors can also be seen in terms of the work of fracture. The work $g_d$ done in each strip (per unit ligament area) until the stress in that strip had been reduced to $0.75\sigma_t$, was computed for each strip. However, many simulations (especially those with shallow notches) were terminated soon after the peak load was reached. In such cases, not many strips achieved the chosen stress limit of $0.75\sigma_t$. The $g_d$ values from sufficiently damaged strips (averaged over the computed realizations, separately for each size and notch depth) are plotted in Fig. 3. The figure shows the crack initiation from a smooth surface to be followed by energy dissipation much larger than that for notched specimen. The energy comparison reveals no gradual transition.

It is also interesting to compare the lattice-particle simulations to the standard cohesive
crack modeling. The macroscopic cohesive law was obtained from stresses $\sigma_x$ and energies $g_d$ measured in strips by the same procedure as introduced in [4]. For each size, a different macroscopic cohesive law was found by averaging the results from 6 realizations with $\alpha_0 = 0.5$. These cohesive laws were then approximated by piecewise linear functions. Then load–CMOD curves were computed for all the notch depths using the pseudo-boundary integral method [1] and piecewise linear approximations.

The maximum loads obtained by the lattice-particle model are compared to the maximum loads from the cohesive crack model in Fig. 4 through relative nominal strength $\sigma_N/\sigma_t$. The nominal strength $\sigma_N$ is defined as the maximal elastic stress in a notch-less beam loaded by peak force $F_{\text{max}}$. Our beam geometry gives $\sigma_N = 90F_{\text{max}}/D$. Assuming that the transition is a deviation from the cohesive crack model, one can see almost no transitional regime in this figure.

Thus we see that the cohesive crack model is close to the lattice-particle model for most of the sizes and notch depths. Only very small sizes and very shallow notches lead to some deviations. However, as already pointed out, these notches have the depth of roughly the minimum aggregate radius and are thus poorly represented in the model. What is clear is that a discrepancy occurs at the zero notch depth, similar to what we concluded from the energy profiles in Fig. 3.

5 VARIATIONS IN DISSIPATED ENERGY

The energy profiles in Fig. 3 show that the energy dissipated up to the point where the stress gets reduced to 0.75$\sigma_t$ depends on the specimen size. Whereas most simulations for $D = 500$ mm give $g_d \approx 20$ N/m, the smaller specimens give lower values. Another systematic, though less visible, decrease of $g_d$ can be seen for increasing notch depths. For the beam sizes of 500, 400 and 300 mm, the relative notch lengths $\alpha_0 = 0.5$ and
0.7 give a lower $g_d$ than the shallower depths. This seems to be a continuous process originating from the width variation of the FPZ; i.e., the wider the zone, the more energy is dissipated.

Visual comparisons of the damaged zone width can be seen in Fig. 5. The smaller the beam size and the deeper the notch, the narrower is the FPZ. Most of the energy is released in the middle of the zone and thus the energy profile comparison makes this dependency less obvious. The size dependence of $g_d$ is also projected into the reconstructed macroscopic cohesive law. The cohesive laws used in the pseudo-boundary integral method in the previous paragraph (and reconstructed for each size from the simulations with $\alpha_0 = 0.5$) are different. The larger the specimen size, the larger are the crack openings for a given cohesive stress.

The conclusions from these numerical simulations broadly agree with experimental observations [10]. The fact that less energy is dissipated as the fracture process gets closer to the upper surface has already been pointed out [11]. Further it appears that the energy dissipation increases as the fracture process gets close to the bottom surface.

6 UNIVERSAL SIZE EFFECT LAW

To describe the dependence of the nominal strength on both i) the relative notch depth $\alpha_0$ and ii) the structure size, $D$, asymptotic matching is useful. The resulting formula, known as the universal size effect law, contained a discontinuity of slope [12, 13, 14, 15]. Here we consider an improved version from which the discontinuity has been removed [16, 17]; it reads:

$$\sigma_N = \left( \frac{E'G_f}{g_0'c_f + g_0D} \right)^{1/2} \left( 1 - \frac{r c_f^2 g_0'' e^{-k\alpha_0^2}}{4(l_p + D)(g_0'c_f + g_0D)} \right)^{1/r}$$

(1)

where $g_0$, $g_0'$, $g_0''$ = values of the dimensionless LEFM energy release function evaluated at $\alpha = \alpha_0$; $g(\alpha_0)$ = square of dimensionless stress intensity factor and its derivative at $\alpha_0$; $E'$
Figure 6: Dependence of nominal strength $\sigma_N$ on relative notch depth $a_0$ and specimen size $D$ obtained by a) lattice-particle simulations and b) analytical formula Eq. (1).

$E$ = effective Young’s modulus; $r$ and $k$ = empirical positive parameters; $l_p$ = approximate width of the FPZ; $c_f$ = material constant, such that $a = a_0 + c_f$ = effective crack length at the peak load. Unlike the present model, which uses a deterministic material strength, the formula can also incorporate the effect of spatial variability of material strength which is the source of the statistical size effect.

To determine the optimal parameters for the type 2 fracture, the Levenberg-Marquardt nonlinear optimization algorithm was used for least-square fitting of the average nominal strength values. Based only on the first part of Eq. (1) and on the nominal strength values for the relative notch depths larger than 0.05, the macroscopic initial fracture energy $G_f = 30.3$ N/m and $c_f = 19.3$ mm was found. The value of $G_f$ corresponds to the initial fracture energy from the reconstructed cohesive law. The value of $c_f$ seems to be rather small, only $0.15l_{ch}$, where $l_{ch} = E'G_f/\sigma^2$ is Irwin’s characteristic length. According to [1], $c_f$ should be about $\pi/24l_{ch}$ for rectangular softening and 0.419$l_{ch}$ for linear softening.

The remaining parameters $l_p$, $k$ and $r$ were found by including the shallower notches and the second part of Eq. (1). But a second least-square fitting yielded unrealistically small values of $r$ and $l_p$ (both were virtually zero). As another approach, it was tried to use realistically chosen values $l_p = 0.01$ m, $k = 300$ and $r = 1/2$. But neither approach was able to fit the nominal strengths provided by the lattice-particle model for zero notch depth. A better agreement for zero notch depth was obtained by considering the entire surface and optimizing all the five parameters $(G_f, c_f, l_p, k, r)$ simultaneously. But such improvement of the fit for a zero notch depth leads to disagreement for the intermediate notch depths; i.e., incorrect $G_f$ and $c_f$ is found.

The two-parameter surface $\sigma_N(D, a_0)$, obtained by averaging the nominal strength values from simulations with the lattice-particle model, is shown in Fig. 6a, whereas the surface given by Eq. (1) for optimized parameter values is shown in Fig. 6b. The averaged simulated nominal strengths are reported in Tab. 1.

The fit by Eq. (1) is also added to Fig. 4. Note that the $\sigma_N$ values from the universal
Table 1: Average values of nominal strength $\sigma_N$ (in MPa) for all specimen sizes and notch depths.

<table>
<thead>
<tr>
<th>$D/\alpha_0$</th>
<th>0.00</th>
<th>0.01</th>
<th>0.02</th>
<th>0.03</th>
<th>0.05</th>
<th>0.10</th>
<th>0.20</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>5.205</td>
<td>5.258</td>
<td>4.931</td>
<td>4.526</td>
<td>3.955</td>
<td>3.257</td>
<td>2.619</td>
</tr>
<tr>
<td>300</td>
<td>4.962</td>
<td>4.005</td>
<td>3.531</td>
<td>3.286</td>
<td>3.067</td>
<td>2.582</td>
<td>2.031</td>
</tr>
<tr>
<td>400</td>
<td>4.746</td>
<td>3.633</td>
<td>3.374</td>
<td>3.019</td>
<td>2.822</td>
<td>2.537</td>
<td>1.832</td>
</tr>
<tr>
<td>500</td>
<td>4.717</td>
<td>3.538</td>
<td>3.227</td>
<td>3.096</td>
<td>2.781</td>
<td>2.268</td>
<td>1.804</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$D/\alpha_0$</th>
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<th>0.40</th>
<th>0.50</th>
<th>0.60</th>
<th>0.70</th>
<th>0.80</th>
<th>0.90</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>2.072</td>
<td>1.457</td>
<td>1.055</td>
<td>0.691</td>
<td>0.387</td>
<td>0.185</td>
<td>0.059</td>
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<tr>
<td>200</td>
<td>1.638</td>
<td>1.302</td>
<td>0.903</td>
<td>0.598</td>
<td>0.349</td>
<td>0.166</td>
<td>0.047</td>
</tr>
<tr>
<td>300</td>
<td>1.549</td>
<td>1.165</td>
<td>0.822</td>
<td>0.541</td>
<td>0.321</td>
<td>0.153</td>
<td>0.043</td>
</tr>
<tr>
<td>400</td>
<td>1.477</td>
<td>1.055</td>
<td>0.767</td>
<td>0.499</td>
<td>0.304</td>
<td>0.144</td>
<td>0.041</td>
</tr>
<tr>
<td>500</td>
<td>1.374</td>
<td>1.024</td>
<td>0.720</td>
<td>0.474</td>
<td>0.283</td>
<td>0.136</td>
<td>0.040</td>
</tr>
</tbody>
</table>

The range of sizes used in the simulations has been quite limited. Because of enormous computational demands, it is difficult to extend the simulations to large beams. Likewise, because of insufficiency of the mesolevel resolution, it is difficult to simulate smaller beams.
with very small relative notch depths, for which a regime of gradual transition might be expected.

The present conclusions should be confirmed by experimental observations. Since any experiments are affected by spatial variability of the local material strength, this variability would have to be incorporated into the present model. This would have to be done in the form of an autocorrelated random field.

8 Acknowledgement

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REFERENCES


STATISTICAL MECHANICS AS GUIDANCE FOR
PARTICLE-BASED COMPUTATIONAL METHODS

IGNACIO G. TEJADA∗ AND RAFAEL JIMENEZ†

∗Dpto. Ingeniería y Morfología del Terreno
Universidad Politécnica de Madrid
C/ Profesor Aranguren, s/n 28040 Madrid (Spain)
e-mail: igtejada@caminos.upm.es/

†ditto.
e-mail: rjimenez@caminos.upm.es

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Abstract. Particle-based methods apply some laws of Classical Mechanics to all the particles of a granular system. On the other hand, classical Statistical Mechanics deals with systems consisting of a lot of particles, focusing on the statistical distribution of some intensive properties. Consequently, the macroscopic behaviour and the average properties of the system in equilibrium are based on some microscopic considerations. To do that, statistical tools and mechanical laws are used together. For an implemented particle-based method to be realistic enough, then the obtained simulations should satisfy some basic underlying physical requirements, and Statistical Mechanics is a useful tool to establish such requirements. This paper presents some results based on Statistical Mechanics that are useful for a realistic modelling of granular systems using Particle-based methods. Examples of the discussed issues include that the same protocol makes a disordered granular medium attain always the same packing ratio; that some local arrangements are less probable than others; that there is a well-established limit to the achievable density of granular assemblies of hard spheres; and that the equilibrium of disordered granular systems does not coincide to the state of minimum potential energy (which would be get in a completely ordered arrangement). The consideration of such issues in practical applications could be helpful to save time in computational methods, to avoid mistakes or, at least, to verify that the implementations are realistic.
1 INTRODUCTION

Engineers are usually concerned about finding which are the stress-strain relationships of granular materials. The complex nature of these media does not make it possible to propose an universal law, or to establish a simple relationship which included all the observed features. In fact, relationships use to be not linear and use to change during static, dynamic and cyclic modifications of the stresses. In consequence many constitutive models have been developed to obtain the stress-strain relationships for jammed granular media by comparing them to special continuum media (macromechanics)[1, 2].

Many of the constitutive equations consider the stress-strain history of the material, which will be decisive for the future behavior. Although today is still a pipe dream finding a universal constitutive law, some results are starting to do it possible for the simplest media. If there was a reproducible state of equilibrium of every medium, it would be possible to propose an equation of state, rather than a constitutive equation [3, 4]. An equation of state is a unique function which relates all the intervening properties of the medium in the equilibrium state. It could be:

\[ f(\text{size distribution, shape, constitutive properties, roughness, arrangement}) = 0 \]

On the other hand, and since the difficulty lies mostly on the complex particular nature of these media, some models focus on the main features of the particles (micromechanics). In particular, since the DEM was proposed by Cundall and Strack [5], particle-based numerical models are being developed. These methods are usually based on the arrangement of virtual individual particles (using simple constitutive equations and solving numerically such equations for the whole interacting system). Saving computational time and ensuring realistic simulations are the aim of a lot of research in this area.

A complement for numerical particle-based methods could be particle-based theoretical approaches. By applying several physical principles, these approaches could be useful to understand some basic properties of granular media. In this paper, an introduction to approaches based on Statistical Mechanics is presented. They are compared to other techniques based on classical mechanics (such as DEM, molecular dynamics, etc.) in Figure 1. Some fundamentals on these techniques are summarized in sections below.

2 FUNDAMENTALS OF STATISTICAL MECHANICS

2.1 WHY USING STATISTICAL MECHANICS?

Thermodynamics studies the conditions of equilibrium and the laws governing the exchanges of various forms of energy or matter of a system which interacts with its surrounding. These laws or principles have been traditionally developed for thermal systems, but they can be applied to other systems, such as granular media.
Figure 1: Comparison between statistical mechanics and classical mechanics approaches of particle-based methods
Statistical mechanics (SM) [6, 7] deals with systems consisting of a lot of particles, describing the macroscopic behavior of systems using microscopic considerations. To do that, statistical tools and mechanical laws are used together. Because granular media consist of a lot of interacting particles, applying these techniques could be interesting.

2.2 DEFINITIONS AND BASIC HYPOTHESIS

Traditionally, statistical mechanics considers physical systems composed of $N$ identical particles confined to a space of volume $V$. Thermodynamic limit conditions means: $N \to \infty$, $V \to \infty$ and $\frac{N}{V} = C$. For granular media, this condition can be probably achieved just imposing that $N \to \infty$ and that the boundary conditions effects are disregarded\(^1\). In this limit, the extensive properties are proportional to the size of the system, $N$, while the intensive properties become independent thereof.

A macrostate of the system is defined according to some macroscopic properties (the state variables), so that if the properties do not change, the macrostate does not change. For instance, the macrostate of a jammed granular system could be described by the number of identical particles $N$ and the elastic potential energy $E$ (which depends on the stresses).

A microstate is a microscopic configuration compatible with a particular macrostate. (For instance, every arrangement of $N$ particles in equilibrium with the stress state of a macrostate).

A given macrostate in general corresponds to a large number of microstates and it is supposed that the system in equilibrium\(^2\) is equally likely to be in any one of these microstates (postulate of equal a priori probabilities). The actual number of possible microstates is expressed as $\Omega(N,E)$.

It is also introduced the ergodic hypothesis: time averages of a system, exploring its mechanically stable states subject to some external drive (e.g., tapping, cyclic stress processes), coincide with suitable ensemble averages over its jammed states. Therefore observing the evolution of a granular system over a driving process for a long time is equivalent to sampling many independent realizations of the same process. The collection of this “mental copies” of the given system is called ensemble. Nevertheless, while for some systems the exploration is produced as time goes by (thermal systems), for dissipative systems (as granular media) energy has to be injected during the driving process.

The phase space $\Gamma$ is the most appropriate workshop for studying the ensembles, by locating the $N$ particles, so that once a particle is placed, its energy is known. The coordinates

\(^1\)For media in which there are particles of different sizes, the thermodynamic limit condition means that, if they are put into groups according to their size $\{N_a, N_b, \cdots\}$, then $N_i \to \infty$ and $N_i/N_j = \text{Constant}$.

\(^2\)Note that every microstate (e. g. every arrangement of a granular medium) is in mechanical equilibrium, but this definition of (thermodynamical) equilibrium relates to the statistical distribution of some intensive properties.
of this space \((q_i, p_i)\) depend on the nature of the intervening energies, while the dimension depends on the number of particles and on the number of degrees of freedom. For instance, to study the motion of \(N\) rigid bodies, the definition of a microstate would require the specification of \(3N\) position coordinates and \(3N\) momentum coordinates, so that the phase space is \(6N\)-dimensional.

The object of Statistical Mechanics is to provide a link between expected macroscopic quantities \(\langle B(\vec{x}, t) \rangle\) (which are fields in the physical space-time) and microscopic quantities \(b(q_i, p_i; \vec{x}, t)\) (which are functions of the phase-space coordinates). This is achieved via the phase-space distribution function \(F(q_i, p_i, \vec{x}, t)\) in the way:

\[
\langle B(\vec{x}, t) \rangle = \int_{\Gamma} b(q_i, p_i; \vec{x}, t) F(q_i, p_i, \vec{x}, t) \, dq_i \, dp_i
\]

### 2.3 Maxwell-Boltzmann Statistics

Different macroscopic environmental constraints lead to different types of ensembles, with particular statistical characteristics. Within the ensembles considered by SM (see [6]), the canonical ensemble is adequate for systems which interact with its surroundings, exchanging energy. Under this consideration, the systems are in equilibrium with an external “reservoir”, and the statistical distribution is governed by a directly observable and controllable parameter (e.g., the temperature for thermal systems). Therefore it is assumed that not all the particles are located at the same energy level, but the distribution is governed by the control parameter of the reservoir.

If the system is non-interacting, then the total energy is given by \(E = \sum_{i=1}^{N} E_i\). If there are \(r\) energy levels and the number of particles which are placed there are \(N_i\) (with \(1 \leq i \leq r\)), then:

\[
N = \sum_{i=1}^{r} N_i \quad E = \sum_{i=1}^{r} N_i E_i
\]

There are a lot of possible multisets \(\{N_i\}\) by means of which the total energy is the same. However, the number of microstates is given by (permutation of a multiset):

\[
\Omega_{(N,E)} = \frac{N!}{N_1!N_2!\cdots N_r!}
\]

According to the postulate of equilibrium, the distribution is obtained by maximizing the equation (3) with the restrictions (2). This can be achieved using Lagrange multipliers and the result is the Maxwell-Boltzmann Statistics [7, 6]:

\[
P_i = \frac{N_i}{N} = \frac{e^{-E_i/\beta}}{\sum_i e^{-E_i/\beta}}
\]

As a result, the distribution depends on \(\beta\), which relates to the control parameter of the surrounding of the system (e.g., the temperature for thermal systems).
Accordingly, it can be demonstrated that for systems of $N$ particles with $S_N$ degrees of freedom, obeying the classical mechanics laws (the Hamiltonian of the whole system is given by $H_{N(q_i,p_i,\alpha)}$), including the external parameters $\alpha$ which have influence on it, a stationary solution which can be reached in equilibrium (corresponding to canonical ensembles) is given by this distribution function:

$$F_{(q,p)} = Z_{N(\beta,\alpha)}^{-1} e^{-H_{N(q_i,p_i,\alpha)}}$$

(5)

where $Z_{N(\beta,\alpha)}$ is called the partition function of the $N$ particles and it is given by

$$Z_{N(\beta,\alpha)} = \int_{\Gamma} e^{-H_{N(q_i,p_i,\alpha)}}\,dp_i\,dq_i$$

(6)

Using (1), the expected value of a variable $B_{(q,p)}$ at equilibrium is given by:

$$< B_{(q,p)} > = \frac{\int_{\Gamma} b_{(q,p)} e^{-H_{N(q_i,p_i,\alpha)}}\,dp_i\,dq_i}{\int_{\Gamma} e^{-H_{N(q_i,p_i,\alpha)}}\,dp_i\,dq_i}$$

(7)

For non-interacting systems, i.e. those systems in which the Hamiltonian is separable $H_{N(q,p,\alpha)} = \sum_{i=1}^{N} H_1(q_i, p_i)$ (so that the total energy is the sum of the individual energies of the particles), it is possible to evaluate the expected value by considering the distribution function of the reduced phase space of just one particle $\Gamma'$, i.e. expression (7) becomes:

$$< B_{(q,p)} > = \frac{\int_{\Gamma'} b_{(q,p)} e^{-H_1(q,p,\alpha)}}{\int_{\Gamma'} e^{-H_1(q,p,\alpha)}}\,dq\,dp$$

(8)

Being $H_1(q,p)$ the Hamiltonian of just one particle.

3 APPLICATION OF STATISTICAL MECHANICS TO GRANULAR MEDIA

3.1 BASIC ASSUMPTIONS

Jammed granular media can be considered as sets of a lot of identical particles interacting via classical forces. The energy exchange with the surroundings is made via the boundary conditions of the elastic problem: external pressures or rigid or deformable walls of the container. As $N$ is very large, the thermodynamic limit condition is assumed. The simplest case is a system consisting of monodisperse (just one diameter size), elastic, cohesionless, frictionless and spherical (3D) or circular (2D) particles. Just a few frameworks based on statistical mechanics have been developed for describing which is the equilibrium state of a granular medium. Two of them are summarized below. They are focused on defining which coordinates make up the phase space and which is the control parameter $\beta$ (it determines the state of the system).
3.2 EDWARDS’ APPROACH

Edwards was the first to propose that a statistical mechanics approach might be feasible to describe dense granular media \[8\]. A new framework was set up to describe the state of powders. Assuming that granular systems have entropy, it was claimed that the volume plays the role of energy.

As a result, a thermodynamic formalism was established based on a phase space which considers the relative position of the particles, a volume functional which takes the place of the Hamiltonian, the effective volume, \( Y \), which is equivalent to the Helmholtz free energy, and a new variable, the frothiness, \( X \), analogous to temperature. This formalism also introduced the hypothesis that time averages of a system, exploring its mechanically stable states subject to some external drive (e.g., tapping), coincide with suitable ensemble averages over its jammed states.

3.3 A NEW APPROACH

Edwards’ theory builds on the idea that particle interactions are produced via hard-core potentials and, as kinetic energy is not taken into consideration, only gravitational energy is (implicitly) considered.

A new proposal \[9\] is based on the idea that the internal stress field (which has to be compatible to the external stress field or the boundary conditions) can be divided in local stress domains. The particles within this stress domains can arrange in several equilibrium configurations and, according to the elastic potential energy, the system is supposed to behave as a canonical ensemble.

In consequence, the energy of a particle of radius \( R \) and (elastic) constitutive parameters \( C_{ijkl} \), arranged according to a configuration \( \alpha \) in equilibrium with a stress field \( \sigma_{ij} \) can be expressed as:

\[
e \simeq \frac{1}{2} \sum_{\alpha} N_{\alpha} \sum_{I=1}^{N_{\alpha}} F_{I,\alpha}(R,\sigma_{ij}) \cdot K_{k,\alpha}(R,C_{ijkl}) = H_{1,\alpha}(R,\sigma_{ij})
\]

(9)

where \( N_{\alpha} \) is the number of coordination of the configuration, \( F_{I,\alpha}(R,\sigma_{ij}) \) are the acting forces and \( K_{k,\alpha}(R,C_{ijkl}) \) is the stiffness of the configuration.

As for a given granular medium, the energy depends just on the stresses and on the arrangement, the phase space is defined by these parameters. Therefore the partition function (6) can be rewritten as:

\[
Z_{1(\beta)} = \sum_{\alpha} \int_{\Gamma_{\alpha}} e^{-\frac{1}{2} \sum_{I=1}^{N_{\alpha}} F_{I,\alpha}(R,\sigma_{ij}) \cdot K_{k,\alpha}(R,C_{ijkl})} d\sigma_{ij} \beta
\]

(10)
Γα is the region of the complete phase space in which every configuration is possible.

Using equation (8) it is possible to obtain the value of any variable depending on the stresses or on the configuration. In particular the packing ratio \( \Phi_{\alpha(\sigma_{ij})} \), which is a function of the configuration and, sometimes, is also function of the stresses. The expression is:

\[
\frac{1}{< \Phi >} = \frac{\sum_{\alpha} \int_{\Gamma_{\alpha}} \frac{1}{\Phi_{\alpha(\sigma_{ij})}} e^{-H_{1,\alpha(\sigma_{ij})}\beta} \, d\sigma_{ij}}{\sum_{\alpha} \int_{\Gamma_{\alpha}} e^{-H_{1,\alpha(\sigma_{ij})}\beta} \, d\sigma_{ij}} \neq f(\beta)
\]

The average compacity does not depend on \( \beta \). It just relates to the volume of the phase space and the stiffness of every possible configuration, which is an intrinsic property of every granular medium.

The parameter \( \beta \) is equal to the inverse average elastic potential energy, i.e. it depends on quadratic functions of the stresses.

\[
\frac{1}{\beta} = \frac{1}{2} \sigma_{\text{ext},ij} S_{\text{eq},ijkl} \sigma_{\text{ext},kl}
\]

being \( S_{\text{eq},ijkl} \) the equivalent compliance tensor of the whole medium. For the case of isotropic compression, an expression to obtain the equivalent volumetric stiffness \( K_{eq} \) is given in [9].

Therefore this new approach allows to obtain the average compacity of the most probable state and other average values of a granular medium just by determining possible equilibrium configurations and by establishing the allowed part of the phase space and the relationship between the stresses and the energy of the particles. For 2D monodisperse systems (the simplest case) and just considering two Crystal-like arrangements, the expected value matches the reported values reasonably (about \( \Phi \approx 0.84 \)-0.86. See [9]).

4 UNDERLYING PRINCIPLES OF GRANULAR MEDIA

4.1 ENERGY AND ENTROPY

The solution of the elastic problem of a conventional continuum medium can be obtained using the techniques of calculus of variations. The potential energy is stationary if the solid is in equilibrium, and furthermore, the equilibrium is stable if the potential energy reaches a minimum (principle of minimum potential energy). This formulation is equivalent to solving the equations of elasticity.

However, if the granular medium is considered as a set of individual particles, this principle is not appropriate because the whole system does not tend to minimize the energy. In fact, the minimum potential energy state (considering both elastic and gravitational
energies) corresponds to the most dense arrangement (a regular lattice for monodisperse media) and, intuitively, this situation is too ordered to be achieved.

Some methods used for modelling the behavior of granular media, as FEMs, use the principle of minimum potential energy but for an approximate continuum medium in which constitutive relationships intrinsically consider particles rearrangement and the consequent variation on the stress-strain behavior. Other methods, as DEMs, apply dynamic and static laws to all the particles. As not only the initial conditions but also the interaction between particles are considered, the resulting state achieved after a calculation can be realistic (and it does not correspond to the minimum potential energy state).

The establishment of the features of the equilibrium state of disordered arrangements could be useful to solve these problems in an alternative way which considers not only the internal energy but also the order. Order and probability are concepts joined by entropy. Boltzmann (1898) [7, 6] proposed that the entropy relates to the number of possible microstates $\Omega$ in the way:

$$S \propto \ln \Omega$$  \hspace{1cm} (13)

Boltzmann went on to show that this definition of entropy was equivalent to the thermodynamic entropy to within a constant number which has since been known as Boltzmann’s constant $k_B$.

However the definition of entropy, which comes from Statistical Mechanics, rather than thermodynamics, is extensible to any system of an ensemble (even when the temperature is not determinant). The entropy is essentially a measure of the number of ways in which a system may be arranged and it is often taken to be a measure of “disorder” (the higher the entropy, the higher the disorder). Thus the definition of entropy given by the Gibb's entropy formula [7, 6]:

$$S \propto - \sum_i P_i \ln P_i$$  \hspace{1cm} (14)

This definition remains valid even when the system is far away from equilibrium. Moreover the 2nd Law of Thermodynamics states that in general the total entropy of any system will not decrease other than by increasing the entropy of some other system, so that the maximization of this quantity states the equilibrium condition.

The observations of disordered granular media evidence that the features of the arrangement are universal and repeatable (if the protocols are the same). This has conducted to the consideration of a kind of entropy of granular media together with the energy state of particles. The equilibrium of disordered granular systems does not coincide with the state of minimum potential energy but with the state of maximum entropy. And overcoming

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3The reason is that entropy is an additive property while probability is multiplicative.
this situation would require the introduction of order to the system, what is less probable. Thus, entropy explains that there is a well-established limit to the achievable density.

This approach could start a new way of solving problems, via describing the most probable state through the maximization of the entropy (14). However, it is important to remark that this minimization gives the state of equilibrium, which is not immediately attained with just a modification of the conditions of the problem. Knowing which is the actual behavior of a granular material after a modification of the conditions is not still possible and to do that a theory of evolution to the equilibrium is necessary.

4.2 THE PROBABILITY OF EVERY ARRANGEMENT AT EQUILIBRIUM

Both approaches included in sections 3.2 and 3.3, show that not all the arrangements are equally likely to be present. The Edward's approach states a distribution function in which the probability of every arrangement depends on the relative volume and on a new property of granular media, the frothiness (which scales the distribution). The new proposal states that the probability of every configuration depends on the volume of the phase space allowed, and on quadratic forms of stresses.

In the equilibrium state, the distribution function of the arrangement is expected to be always the same so this is an underlying principle which had to be satisfied. On the other hand, statistical mechanics approaches could be useful for the establishment of some patterns of assemblies in equilibrium.

This considerations could be helpful for the first step in discrete element simulations: the generation of the initial assembly. Nevertheless, preparing an initial distribution of a large number of particles in a realistic and random-like manner is not trivial and it concerns to a lot of researchers.

Two kinds of methods for the preparation of dense arrangements for simulations are possible (for a review, see [10]): dynamic methods (or non-constructive) and constructive algorithms. Dynamic methods use the DEM code itself for the preparation of the sample, by different ways: increasing diameters, moving slowly the walls of the domain (and allowing particles to be rearranged) or by gravitational deposition; constructive methods are less time-consuming and their basic feature is that assemblies are prepared with the help of purely geometrical calculations, without simulating the dynamics of particle motion.

Additional techniques to generate realistic initial samples, as well as the need to develop appropriate algorithms have been highlighted by some researchers [11, 12] However, it is not definitely well-established what is a good sample. Probably the distinction depends on the desired precision. Apparently, engineers are more concerned about the time consumed to obtain a dense arrangement (within a precision range of about 1%). On the other hand, physicists are concerned about the definition of the ground state of granular
media (arising concepts as random close and random loose packing).

Starting from the hypothesis that identical granular media (i.e. those described by the same particle shape and size distribution, friction factor, and other parameters) give the same response to the same protocol of arrangement, statistical mechanics approaches try to define the macroscopic features which the system attains. These approaches differentiate equilibrium states (described by an equation of state) and states out of equilibrium (which would be more or less sensible to external driving and which would tend to the equilibrium situation). In consequence, they could illuminate how likely is every generated arrangement. Moreover, if those arrangements corresponding to the equilibrium state were defined, we could avoid the generation of initial assemblies in every simulation.

4.3 THE MOST PROBABLE AVERAGE PACKING RATIO

Once the distribution function of the phase space is known, the average value of variables which depend on the phase space coordinates can be computed using (8). According to the approach mentioned above, the expected packing ratio at equilibrium is given by (11) and it does not depend on $\beta$. This lead us to the conclusion that the expected value of the density of a granular medium is not affected by the stress level but by whether the system is in equilibrium or not. Therefore $\Phi$ is an intrinsic property of the medium (which depends on the shape, size-distribution and friction of particles). Although granular media can be found in looser or denser configurations, driving the system (by tapping or cyclic compression, for instance) would make it to tend towards the equilibrium state. However, once this situation has been reached, the same process does not make it to abandon that state (that would require the introduction of order into the system). This reasoning can be helpful to explain some concepts, such as random close packing and evidences why granular systems always tend to attain close values of packing ratio. Nevertheless, some experimental results have shown that the attained average packing ratio depends on the protocol used to configure the arrangement. This is probably due to the fact that the equilibrium state is not always totally reached. Although this is still an open question, the relative differences among reached states are mostly within the desired precision for engineering purposes.

If the equilibrium state of a granular medium is determined, the variations of the average packing ratio (and other properties) could be determined by the analysis of the evolution from initial (out of equilibrium) states to the equilibrium state. Nevertheless a proper framework has to be developed.

5 CONCLUSION

Statistical Mechanics could be an useful tool to explain certain aspects of the behavior of granular materials.
First results have shown that these analytical particle-based methods could complement other numerical particle-based techniques (such as DEM or Molecular Dynamics) or continuum models (used in FE and Finite Difference Methods). Consideration of these results could be useful for the generation of initial arrangements and the analysis of the evolution towards the equilibrium situation, although more research is still needed to establish a complete framework for the analysis of several media. In such research numerical results and theoretical developments should be performed at the same time.

REFERENCES


THE EFFECTS OF ROLLING RESISTANCE ON THE STRESS-STRAIN AND STRAIN LOCALIZATION BEHAVIOR OF GRANULAR MATERIALS DUE TO SIMPLE SHEAR LOADING CONDITIONS.

Abdalsalam M. Muftah* and Marte S. Gutierrez†

Colorado School of Mines/Division of Engineering (CSM)
1610 Illinois St., BB 269. Golden, CO 80401, USA
*Corresponding author (e-mail: amuftah@mines.edu)

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1 INTRODUCTION

The previous studies has conclusively shown that rolling resistance is a significant parameter influencing the stress-strain and strain localization response of granular materials when a failure state can be reached in biaxial test with small strain, (2-4%) of axial strain [1, 2]. However, in order to allow for larger deformations, numerical experiments are carried out for a simple shear test. In these simulations strain localization can be obtained for relatively high shear strain. The main objective of this paper is to present the results of a comprehensive study using DEM modeling of the effects of the variation in rolling resistance on the elasticity, shear strength, dilation and bifurcation response of granular materials subjected to simple shear loading. A comprehensive parametric study is performed whereby the magnitude of rolling resistance is varied within its full range of possible values in conjunction with variations in other model parameters, and more practically to interpret the macroscopic behavior of granular specimens subjected to different loading conditions from the viewpoint of micromechanics.

To this end, a DEM Model using the Particle Flow Code in two dimensions (PFC2D) is put forward to study localization phenomenon of granular material in simple shear test. A detailed analysis of this numerical test in view of microstructure of shear band, as regards the effect of the rolling resistance parameters on stress-strain, dilation, and other shear band features will be investigated. This objective of study is to take a close look at the deformation process by means of micro structural observation which may help to analyze the macro structural of shear bands.

2 DEM MODELING

The initial state of the DEM sample is performed under two-dimensional simple shear loading conditions. The simple shear model is rectangular, 0.06 m high and 0.12 m wide, and consists of an assembly of poly-dispersed disk-like particles (see Fig.1). Three ranges of particle radii were used: 0.3-0.4 mm, 0.3-0.6 mm and 0.3-0.8 mm. For these particle radii, the size of the model is deemed large enough to simulate a representative element volume of
granular material, but not too large to require extensive calculation times. The sample is contained by four frictionless walls. The top and bottom boundaries are confined by rigid platens and by the vertical normal stress $\sigma_1$. The left and right lateral walls are confined by semi-rigid walls and by the minor principal stress $\sigma_3$. The sample is first loaded isotropically during consolidation, then sheared by rotating the vertical walls at a constant angular velocity about the mid-points of the two walls, then increased the rotated velocity until the peak and post peak shear stress have been achieved. Shearing is performed under constant angular velocity $d\gamma / dt$ of 0.05 m/min and constant vertical normal stress. The vertical walls rotate towards the right direction under an angular velocity controlled condition.

The velocity of the horizontal walls is controlled automatically by a numerical servo-control program that maintains that the vertical normal stress component of the stress tensor does not change from the initial value. To generate the model, a random particle generation procedure called the “expansion method” [3] is adapted to achieve a desired sample particle size distribution and porosity. The expansion method employs a constant factor, expressed as a multiple of the particle radii, which is adjusted and the particle sizes are increased until the system reaches an equilibrium state after some calculation cycles. Due to the particle radii expansion, particles greatly overlap and thus strong repulsive forces are developed at the contacts. Cycling is required to achieve equilibrium between the unbalanced forces and the forces generated by the isotropic boundary stresses from consolidation.

The model parameters values used in the study are summarized in Table 1. The material parameters (i.e., density $\rho$, normal stiffness $K_n$ and friction coefficient $\mu$) are similar to those used by [4] in the DEM simulation of the stress-strain behavior of granular materials. Some of the parameters were given a range of values to test the sensitivity of model response to changes in parameter values. The lateral walls were given a stiffness that is $1/10^6$ of the particle-to-particle contact stiffness in order to simulate a semi-rigid confining membrane. The simple shear tests were run for range of vertical normal stress with $\sigma_1$ varying from 0.1 to 2 MPa. It is known in the literature that a DEM model with more than 5000 particles provides a representative element volume for the modeling of the stress-strain response of granular materials.

![Figure 1](image1.png)

**Figure 1.** Set-up of the simple shear DEM model for the simulation of the stress-strain and strain localization response of granular materials.
materials. In this study, the number of randomly generated particles ranged from 6556 to 16190 (see Table 1).

Table 1: Model parameter values used in the DEM simulations.

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample Dimensions (cm)</td>
<td>Height: 6, Width: 12</td>
</tr>
<tr>
<td>Particles Sizes (mm)</td>
<td>0.3 – 0.4, 0.3 – 0.6, 0.3 – 0.8</td>
</tr>
<tr>
<td>Number of Particles</td>
<td>16190, 9794, 6556</td>
</tr>
<tr>
<td>Porosity, ( n )</td>
<td>0.10, 0.13, 0.16</td>
</tr>
<tr>
<td>Particle Density, ( \rho ) (kg/m³)</td>
<td>2630</td>
</tr>
<tr>
<td>Inter-particle Friction Coefficient, ( \mu )</td>
<td>0.5, 0.6, 0.7</td>
</tr>
<tr>
<td>Contact Normal Stiffness, ( K_n (N/m) )</td>
<td>(5 \times 10^8)</td>
</tr>
<tr>
<td>Ratio of Shear and Normal Stiffnesses, ( K_s / K_n )</td>
<td>1.0</td>
</tr>
<tr>
<td>Wall Stiffness, ( K_w (N/m) )</td>
<td>(5 \times 10^7)</td>
</tr>
<tr>
<td>Particle Rolling Resistance, ( \alpha )</td>
<td>0.0, 0.01, 0.1, 0.5, 1.0</td>
</tr>
<tr>
<td>Confining Stress, ( \sigma_1 ) (MPa)</td>
<td>0.1, 0.8, 2.0</td>
</tr>
</tbody>
</table>

The rolling resistance parameter \( \alpha \) is affected by the particle shape, normal stiffness and normal force at a point of contact and its value typically ranges from 0 to 1. For \( \alpha = 0 \), no rolling resistance (i.e., free rolling) exists at a contact point. Based on a preliminary analysis, particle rotation is effectively prevented (i.e., no rolling) when \( \alpha = 1 \). As noted above, \( \alpha \) is analogous to the friction coefficient \( \mu \) and, thus, a value of \( \alpha = 1 \) is equivalent to prescribing a high rolling friction angle of 45°. Therefore, parameter \( \alpha \) is given values between 0 and 1 in the simulations presented below. Table 1 lists the specific values of \( \alpha \) in conjunction with the other model parameters used in the simulations.

3 STRAIN TENSOR AND MESH-FREE METHOD

To quantify strain localization and shear banding behavior and calculating shear strain distribution inside the shear box. A new simple method of strain calculation has been developed by [5], and used in this study to generate strain field inside a simulated simple shear box. A modified mesh-free method calculates the displacement gradient directly based on movements of individual particles. This method accounts for particle rotation and captures strain localization features at high resolution. For the current problem involving large strain localization inside the granular medium, the Green-St Venant strain tensor \( E_{ij} \) can be expressed as:

\[
E_{ij} = \frac{1}{2} (u_{ij} + u_{ji} + u_{ij}u_{ji})
\]  

(1)

Where \( u_{ij} \) is the displacement gradient tensor. It is based on the deformation measure related to the reference configuration. For peak or pre-peak shear deformation involving slight degree of strain localization, the second-order term in Eq. 1 can be neglected with little error, and the small tensor \( e_{ij} \) is computed by:
\[ E_{ij} = \frac{1}{2} (u_{ij} + u_{ji}) \]  \hspace{1cm} (2)

The mesh-free method used in this study employs a grid-type discretisation over the reference configuration. The spacing between adjacent grid points used in this study is 0.45 mm in the horizontal direction and 0.45 mm in vertical direction. As a general guide, a grid spacing of the median particle diameter \( d_{50} \) is sufficient to capture the shear localization at satisfactory resolution. A diagram of the approach is given in Fig. 2 where a rectangular grid is superimposed over the volume of particles prior to any deformation and serves as the continuum reference space. Then each grid point in the reference space is assigned to an individual particle \( p \) that has the property.

\[ \frac{d_i}{r_j} \leq \frac{d_i}{r_i} \quad (i = 1, 2, \ldots, N_p) \quad i \neq j \]  \hspace{1cm} (3)

Where \( r_j \) is the radius of particle \( i \), \( d_i \) is the distance between the grid point and the centroid of particle \( i \); and \( N_p \) is the total number of particles within the volume (see Fig. 2a). If the ratio of the distance between the particle centroid and its associated grid point to the particle radius is the least among all the particles, then the grid point is considered a point on the rigid or extended body of the particle. In fact, any point (not necessarily the grid point) inside the volume can be assigned to a particular particle using Eq. 3. All points that are assigned to a given single particle are then connected to form a region that belongs to this particle. Displacement of the grid point is calculated using the principal of rigid body motion of the particle.

\[ \begin{pmatrix} u_x^g \\ u_y^g \end{pmatrix} = \begin{pmatrix} u_x^p \\ u_y^p \end{pmatrix} + d \begin{pmatrix} \cos(\theta_o + \omega) + \cos(\theta_o) \\ \sin(\theta_o + \omega) + \sin(\theta_o) \end{pmatrix} \]  \hspace{1cm} (4)

Where \( u_x^g, u_y^g \) and \( u_x^p, u_y^p \) are the \( x \) and \( y \) components of displacement of grid point and particle centroid respectively; \( d \) is the distance between the grid point and the particle centroid, \( \theta_o \) is the initial phase angle of the grid point position relative to the particle centroid; and \( \omega \) is the accumulated rotation of the particle (see Fig. 2b). The displacement of any point inside the volume can be uniquely determined using this method; therefore a unique strain tensor is
obtained at any stage of the simulation. This method also takes into account the particle rotation; therefore it is able to capture accurately the actual strains that the granular media is experiencing.

4 RESULTS AND DISCUSSION

4.1 Effects of Rolling Resistance on Elastic Behavior

The stress-strain response of the modeled granular material subjected to simple shear loading conditions are shown in terms of the shear stress ratio $\tau / \sigma_n$ vs. shear strain $\gamma_{xy}$ curves in Fig. 3a for different values of the rolling friction coefficient $\alpha$. Except for $\alpha$, all other values of the model parameters, vertical normal stresses and initial porosities are kept the same and these values are given in Table 1. It can be seen that the initial slopes of the stress-strain curves are identical for all values of $\alpha$. It appears that the Young’s modulus of the modeled granular material is not affected by the rolling resistance. This observation is in agreement with that of [6, 7].

Figure 3b shows the volumetric strain $\varepsilon_v$ vs. shear strain $\gamma_{xy}$ response of the modeled granular material as a function of $\alpha$ corresponding to the shear stress-strain response curves (see Fig. 3a). The volumetric strain increment is defined as $d\varepsilon_v = d\varepsilon_x + d\varepsilon_y$ where $d\varepsilon_y$ is the corresponding increment in the vertical dimension of the sample, which there is no change in the horizontal dimension $\varepsilon_x$. Like the $\tau / \sigma_n$ vs. $\gamma_{xy}$ curves, the initial portions of the $\varepsilon_v$ vs. $\gamma_{xy}$ and $\tau / \sigma_n$ vs. $\gamma_{xy}$ curves are very similar and are unaffected by the rolling friction coefficient. This indicates that the elastic Poisson’s ratio $\nu$ of the modeled granular material is independent of $\alpha$.

![Figure 3](image_url)

Figure 3 Effects of the rolling friction coefficient $\alpha$ on the (a) shear stress-strain and (b) volumetric strain response of granular materials under simple shear loading condition.

4.2 Effects of Rolling Resistance on Shear Strength and Dilatancy

In contrast to the initial state of shear stress ratio and dilatancy curves, it was found that the particle rolling resistance coefficients $\alpha$ played an important role in the movement of these curves of the granular specimens after bifurcation points (Figs. 3 and 4). From Fig. 3a, it can be clearly observed that an increase in the rolling friction coefficient $\alpha$ results in higher peak...
strength. The peak shear stress ratio is increased from 0.4 to 0.57 when \( \alpha \) is increased from 0 to 1. The increase in peak shear stress ratio with increasing \( \alpha \) indicates that rolling resistance increases the overall frictional resistance of the granular material. The peak shear stress ratio also occurs at higher shear strains for high values of \( \alpha \) compared to the stress-strain response at low values of \( \alpha \). In addition, strain softening curves show a small amount of softening in post-peak shear stress for all values of \( \alpha \). It worth noting that high value of \( \alpha \) is, small amount of softening can be increased. Figure 4a shows that the residual states are similar for granular specimens subjected to different confining stresses and the same values of \( \alpha \), whereas Figure 4b shows that granular specimens subjected to higher confining stress have lower volumetric dilation in volumetric strain curves.

As observed in Fig. 3b, as the shear strain is increased, the simulated materials with free rotation or with rolling resistance undergo lower volumetric contraction and start to dilate at an earlier stage with \( \varepsilon_1 = 1\% \) compared to the materials shearing under biaxial loading condition [1]. The dilative volumetric strain increases as the rolling resistance is increased. The increased dilative volumetric changes for the models with high \( \alpha \)-values is attributed to the fact that the increased moment between particles caused by the rolling resistance results in the particles being pushed from each other during shearing. On the other hand, in the models with low rolling resistance, the particles are free to jostle around and accommodate each other resulting in smaller dilation. Tordesillas [8] presented similar results indicating that dilatancy increases with increasing rolling resistance.

\[ \sin(\theta_s) = \left( \frac{\sigma_1 - \sigma_3}{\sigma_1 + \sigma_3} \right)_{\max} \]  

Figure 5 summarizes the effects of the rolling friction coefficient \( \alpha \) on the peak secant friction angle \( \theta_s \), which is defined as:

For a friction coefficient of \( \mu = 0.6 \), the secant friction angle \( \theta_s \) continuously increases from about 24° for \( \alpha = 0 \) to about 35° for \( \alpha = 1 \) (see Fig. 5a). The most significant increase in the secant friction angle occurs for \( \alpha < 0.15 \), and for \( \alpha > 0.15 \) the change in the friction angle is very small. The variation of the \( \theta_s \) as function of \( \alpha \) is similar for three values of \( \mu \): 0.5, 0.6 and 0.7. In general, for the same \( \alpha \)-value, the peak secant friction angle increases with an increase in the
friction coefficient $\mu$. Figure 5b shows the combined effects of $\alpha$ and the vertical normal stress $\sigma_1$ on the secant friction angle $\phi_s$.

![Figure 5](image-url) Effects of the rolling friction coefficient $\alpha$ on peak secant friction angle (a) as function of friction coefficient $\mu$ and (b) vertical normal stress $\sigma_1$.

Similar to Fig. 5a, the secant friction angle $\phi_s$ changes dramatically for $\alpha<0.15$, and very little change occurs when $\alpha>0.15$ for all $\sigma_1$-values. As expected, for the same value of $\alpha$, the secant friction angle $\phi_s$ decreases with increasing confining stress $\sigma_1$.

Figure 6 shows the effects of rolling friction coefficient $\alpha$ on the peak dilation angle $\varphi$, which is defined as:

$$\sin(\varphi) = \frac{(\frac{d\varepsilon_1 + d\varepsilon_3}{d\varepsilon_1 - d\varepsilon_3})_{\text{max}}}{(d\varepsilon_\nu/d\varepsilon_1)_{\text{max}}^2}$$  \hspace{1cm} (6)

In general, the dilation angle $\varphi$ increases for $\alpha \leq 0.15$ then decreases afterwards. For instance, for the friction coefficient of $\mu = 0.6$, the dilation angle $\varphi$ increases from its lowest value of about $12.5^\circ$ for $\alpha = 0.0$ to a maximum of about $20^\circ$ for $\alpha = 0.15$, then decreases to $15^\circ$ for $\alpha = 1.0$. The same variation of $\varphi$ with respect to $\alpha$, is observed for different values of $\mu$ (Fig. 6a), and for different values of $\sigma_1$ (Fig. 6b). For the same $\alpha$-value, the dilation angle increases with increasing $\mu$ (Fig. 3.6a) and decreases with increasing confining stress $\sigma_1$ (Fig. 6b).
4.3 Effect of Rolling Resistance on Shear Band Orientation

To further quantify the effects of rolling resistance on shear band formation, the orientations of the shear bands were directly measured from the models. Only the cases with distinctly observable shear bands were included in the analysis. It was observed that the shear bands were not always completely straight along its length, but sometimes tend to bend towards the corners of the four edges of the samples. Thus, the shear bands were measured along the straight line portions of the shear bands in the middle of sample. The orientations of the shear band plane $\theta_m$ from the models were measured from the horizontal axis, and these are shown against $\alpha$ in Fig. 7. The measured shear band inclinations are compared with three theoretical shear band orientations. These are the Mohr-Coulomb orientation $\theta_{MC}$ and Roscoe orientation $\theta_R$ [9] which is, respectively, the upper and lower bound values of the orientation of the shear band plane measured from the horizontal axis (Eqs. 3 and 4). The third orientation is the Arthur-Vardoulakis orientation $\theta_{AV}$ from [10, 11] which corresponds to the average inclination between the Mohr-Coulomb and Roscoe orientations (Eq. 5). Figure 7 shows the variation of the measured shear band orientation $\theta_m$ from the models against the rolling friction coefficient $\alpha$. It is observed that $\theta_m$ first increases with increasing value of $\alpha$. The measured shear band inclination angle for free rotation is about $\theta_m = 55^0$, then it reaches its highest value at about $\theta_m = 58^0$ at $\alpha=0.1$ and decreases thereafter to $\theta_m = 57^0$ for $\alpha=1.0$. 

Figure 6 Effects of the rolling friction coefficient $\alpha$ on peak dilation angle (a) as function of friction coefficient $\mu$ and (b) vertical normal stress $\sigma_t$. 

![Figure 6](image-url)
Figure 7 Effects of the rolling friction coefficient $\alpha$ on shear band orientation

Figure 7 also shows the Mohr-Coulomb, Roscoe and Arthur-Vardoulakis shear band orientations from Eqs. 4 and 5 using the measured peak friction angle $\varphi$ and dilation angle $\psi$ from the models. The measured shear band orientations are located between the Arthur-Vardoulakis and Mohr-Coulomb orientation predictions. The Mohr-Coulomb orientation over predicts while the Arthur-Vardoulakis orientation under predicts the measured shear band inclinations. Similar variation of shear band orientation as function of $\alpha$, were observed for different particle sizes and values of the friction coefficient $\mu$ and confining stress $\sigma_3$.

4.5 Micromechanical Observations

One of interesting features that arise from micromechanics analysis is the formation of force chains which are considered the primary load carrying mechanism of granular materials [10], where the contact force between them is rather stronger than the other force outside particle chains. Force chains are quasilinear arrangements of groups of particles by which almost all the shear loads are transmitted. Their average orientations are more or less sub-parallel to the major principal stress, and they form solid column-like structures in order to resist the shear stress and insure stability of granular materials. When a granular assembly is loaded and sheared, force chains form, rotate and collapse as the shearing progresses. Force chains develop anisotropically during shearing due the fact that not all particles are selected to form force chains. As the shearing proceeds beyond peak shear stress, the major force chains reorganize until they can no longer provide the best possible set of stress pathways for force transmission.

The reconfiguration of force chain networks for granular assembly subjected to simple shear loading is associated with the rotation of principal stress. The direction of force chain is consistent with the rotated stresses. Before shear loading, the network of force chains is dense and evenly distributed with no preferred directions throughout the volume of the granular materials (see Fig. 8a). Once the granular assembly is loaded, all pathways can be developed into strong and weak force chains as they formed to transmit the shearing loading. The key feature of simple shear condition during shearing is associated with the principal stress rotation. Therefore, the microstructure of force chains undergoes sub parallel with the rotated
principal stresses (see Fig. 8b). Once the peak shear stress is reached, the density of the number of force chains is reduced inside the shear band, and there are fewer particle-to-particle contacts available within the shear band to transmit the loads.

As the number of particle contacts is decreased, the shear loading may exceed the frictional resistance between particles causing the force chain to collapse, limitation of force chain collapsing leads localization of strain (see Fig. 8c). As the shearing proceeds beyond peak shear stress, shearing process leads to the exhaustion of the strength of the material. As a result, the load carrying capacity of granular materials is reduced and strain softening occurs [12]. Due to the deviation of the force chain directions from the major principal stress direction, high rotational moments and stress gradients were produced within the shear band. Instability and strain localization occurred due to the changes in configuration of the force chains and the presence of rotational moments and stress gradients. In the case of $\alpha=0$, particles rotated widely over the granular assembly at all stages of deformation. In comparison, in the case of rolling resistance, the particles showed only very small rotations before the shear band was formed.

Once deformations have localized, particle rotation occurred extensively within the shear band while no significant rotations were observed for the particles outside the shear band. As a result, the shear band formation was accompanied by gradients in the magnitude of particle rotations. Particle rotation within the shear band in the presence of rolling resistance was associated with the formation of non-uniform void distribution within the shear band. Paradoxically, large voids were created at the same time that the shear band width decreased as $\alpha$ is increased. The occurrence of areas of large voids where particles have high rolling resistance was attributed to the fact that particles, in the presence of rotational moments, tended to push each other apart. This caused the granular assembly to expand and increase the porosity locally. In comparison, particles were free to move and accommodate each other, resulting in more uniform void distribution.

4.6 Strain Localization inside the Shear Band

The development of strain localization can be better evaluated by the shear strain contours show in Fig. 9. The shear strain $e_{ij}$ value is calculated using the proposed strain calculation method (Eq. 2), using the mesh-free method. A series of micro bands emerge in a sequential way to form the final shear band. Results show that the shearing condition inside the granular specimen during initial conditions is assumed to be uniform. Hence, there is not any sign of strain localization existence (Fig. 9a). As shearing proceeds, some shear distortion has occurred at pre failure $\gamma_{xy}=0.13$, indicating the plastic shear band extends over the length at the
middle plane propagating straight in the horizontal direction. Meanwhile, nonlinear stress-strain behavior marks the effective start of plastic regime and the onset of shear band would become. The shear band in this stage cannot be seen clearly in Fig. 9b due to the resolution of the plot. A fairly small and uniform strain field can be found inside granular assembly as a plastic flow confined between two semi-rigid plates moving in opposition directions. After peak state, the shear band expands and becomes expansive and coherent with post peak strain softening immediately after failure $\gamma_{xy} = 0.16$. The peak of the mound is located approximately at the middle of the shear box, with a width of about 18 median particle diameters thick (Fig. 9c). During the processes of strain localization, not only the shear strain increases but also the volumetric strain is locally increased due to localized dilatancy. At steady state $\gamma_{xy} = 0.38$, a distinct shear band is observed which becomes continuous, cumulative and thicker, dividing the shear box into two halves. However, the contour plot clearly shows that the strain localization is fully developed (Fig. 9d). The thickness of the strain localization zone was almost 10-20 times the median particle diameter $D_{50}$ on the average and increase generally with increasing of shear strain. The increase in dilation is attributed to the increase of the interface between particles and the subsequent increase in the shear band thickness.

![Figure 9 Shear band formations inside dense sample corresponding simple shear loading.](image)

5 CONCLUSIONS

This work presents an extensive investigation of the effects of rolling resistance on macro behavior of granular specimens subjected to simple shear loading conditions using DEM modeling. The Modified DEM implemented a rolling resistance model in PFC. The results concluded that the Young’s modulus $E$ and Poisson’s ratio $\nu$ were relatively unaffected by the rolling friction coefficient $\alpha$. The peak secant friction and dilation angles increased with increasing value of the rolling friction coefficient $\alpha$. Once deformations have localized, particle rotation occurred extensively within the shear band while no significant rotations were observed for the particles outside the shear band. Particle rotation within the shear band in the presence of rolling resistance was associated with the formation of non-uniform void distribution within the shear band. The shear strain contours developed using the mesh-free method, indicating that strain localization does not exist during initial conditions. As shearing proceeds, the shear band thickness expanded and became thicker and generally increased with increasing shear strain. This observation is attributed to the increase in local softening and dilation inside shear localization zone.
REFERENCES


3D VIRTUAL LABORATORY FOR GEOTECHNICAL APPLICATIONS: ANOTHER PERSPECTIVE

V. ROUBTSOVA*, M. CHEKIRED*, B. MORIN*, and M. KARRAY†

* Hydro-Quebec Research Institute
1800, boul. Lionel-Boulet, Varennes (Québec)
Canada J3X 1S1
bureau.accueil@ireq.ca, www.ireq.ca

† Université de Sherbrooke
Department of Civil Engineering, Faculty of Applied Sciences
2500 boulevard de l’Université, Sherbrooke (Québec)
Canada J1K 2R1
mourad.karray@usherbrooke.ca, www.usherbrooke.ca/gcivil/

Key Words: DEM, Cohesionless Soils, Shear Tests, OpenCL, OpenGL, Alioscopy.

Abstract.

Discrete element methods are important tools for investigating the mechanics of granular materials. In two dimensions, the reliability of these numerical approaches is increasingly being challenged, because they cannot take into account all the factors involved in the behavior of a granular medium.

With new concepts, such as high performance parallel computing and 3D visualization, it is now possible to conduct numerical simulations of granular materials made up of several thousands of particles, and also to follow the evolution of the various parameters involved in the behavior of a granular medium. Experimental tests have been carried out to validate the results obtained by using a virtual laboratory. This paper presents the earlier results obtained in our 3D Virtual Laboratory on the response of specimens of glass beads of uniform size during shear tests. Good agreement was achieved between the virtual simulations and the experimental tests.

This work highlights the possibility of using a new 3D virtual laboratory for dynamic simulation. This approach could be of significant value in improving the verification, validation, and communication of the simulation results of discrete element methods, which can in turn make the simulations more credible and thus useful in decision making.
1 INTRODUCTION

The direct shear test is widely used to measure the bulk material properties required to design many engineering problems, such as foundations, retaining walls, slab bridges, pipes, sheet piling, etc. Several attempts to numerically model this test in 2D have been conducted. However, the results obtained to date have often been marred by uncertainty, and so this 2D approach is not yet widely used. In addition, attempts are rarely made to validate the experimental results obtained by numerical modeling, and have often not been conclusive enough to impress practitioners. Computer hardware limitations have also slowed its widespread acceptance. In order to overcome these difficulties, a parallel computation approach has been used to develop a dynamic 3D numerical code (called SIMSols). The OpenCL framework was used in order to achieve a high level of data parallelism on NVIDIA Graphics Processing Unit (GPU) based Tesla High Performance Computing (HPC) hardware. Using the OpenGL Application Programming Interface (API) and Alioscopy technology, autostereoscopic visualization is proposed. This paper presents the results obtained experimentally on a series of shear tests carried out on samples made up of glass beads, which helped validate the virtual laboratory results.

2 DIRECT SHEAR TEST

The direct shear test is one of the oldest soil strength tests performed in the laboratory. Even though this test has some disadvantages, which are documented in ASTM D 3080 – 98 [1], this test is routinely used by geotechnical engineers to determine the shear strength parameters of soil that are essential for stability assessment. The first direct shear apparatus was built by Alexander Collin in 1846 to measure the strength of a clay soil shear to study the stability of slopes [2, 3, 4]. The current version of the direct shear apparatus was designed by Casagrande in 1932.

A normal load is applied to the specimen and the specimen is sheared across the predetermined horizontal plane between the two halves of the shear box. Measurements of shear load, shear displacement and normal displacement are recorded. From the results, the shear strength parameters can be determined. Figure 1 shows a schematic representation of the shear box.

![Schematic representation of a shear box](image.png)

**Figure 1:** Schematic representation of a shear box
3 DISCRETE ELEMENT METHOD SIMULATIONS

The Discrete Element Method (DEM), proposed by Cundall and Strack [5], is a powerful tool for numerical modeling of the mechanical behaviour of a large number of particles. Each particle is considered as a rigid body with translational and rotational degrees of freedom assigned to their centers of mass. An explicit time integration scheme, based on Newton’s second law, is applied to the equations of motion to keep track of the particle positions and velocities. While moving, some of the particles will come into contact with one another. To address this issue, a contact formulation is required to apply repulsive forces to prevent the particles from moving through each other.

In spite of the progress made to date, practitioners in fields such as granular materials science, geotechnical, mining, the food industry, etc. still lack confidence in this method, and, as a result, further development is required. In the geotechnical field, for example, the major concern is the prohibitive computational time it requires, and another is the non-representativeness of the 2D approach in evaluating the various phenomena encountered in dense granular materials. In fact, modeling 2D fails to take into account all of the involved parameters. This has been confirmed by several studies, including that of Sallam [6], who observed that the dilatancy of the 2D model is greater than that observed experimentally. Sallam attributes this difference to the fact that, in 2D simulations, particles cannot benefit from the level of freedom that 3D offers. In terms of the contact between particles, Masson et and Martinez [7] simulated granular material confined in a gallery and subjected to a horizontal thrust. Their simulation was conducted in both 2D and 3D. The results show that the 3D model allows a compaction and displays significantly more contacts than a 2D model. On the other hand, by comparing experimental results on Daytona Beach sand and on rounded materials with those obtained by numerical simulations, Das [8] found that the 2D simulations underestimate the results for both materials. The angle of internal friction of Daytona Beach sand obtained from 2D simulations was 27°, while that obtained from 3D simulations varies from 39 to 43°, which is close to the experimental value of 37.40°. For rounded materials, the angle of internal friction obtained from 2D simulations was 17.2°, while that obtained from 3D simulations varies from 25° to 26.6°, which is within the internal friction angle range of 24.4° to 27°, as reported in the literature by O'Sullivan et al. [9] and Phillips et al. [10].

Finally, while there are numerous publications describing the potential of DEM, only a small number of studies in the geotechnical field have been validated by experimental results [11].

A further concern is particle shape. It is well known that the geometry of real soil particles is not adequately represented by spheres, and that samples formed of spherical particles cannot represent the complexity of soil behavior. Attempts to simulate soils with particles of simple non-spherical form in 2D began to be considered in the last decade [6, 12] and in 3D [13, 14].
4 THE MOTION AND INTERACTION OF PARTICLES (DEM)

The motions of particle \( i \) caused by its interactions with neighbouring particles is described by the equations:

\[
\begin{align*}
    m_i \frac{d\vec{V}_i}{dt} &= m_i \vec{g} + \sum_{j=1}^{k} \left( F_{cn,i,j} + F_{dn,i,j} + F_{ct,i,j} + F_{dt,i,j} \right) + F_{fl} \\
    I_i \frac{d\vec{\omega}_i}{dt} &= \sum_{j=1}^{k} \left( \vec{T}_{ij} + \vec{M}_y \right) + \vec{\Phi}_f
\end{align*}
\]

(1)

where:

- \( m_i \) and \( I_i \) are the mass (kg) and moment of inertia (kg.m\(^2\)) of particle \( i \) respectively;
- \( \vec{V}_i \) and \( \vec{\omega}_i \) are the translational (m/s) and rotational (s\(^{-1}\)) velocities of particle \( i \) respectively;
- \( k \) is the number of neighboring particles;
- \( F_{cn,i,j} = -K_n \delta_n \vec{n} \) is the normal force of contact (N);
- \( F_{dn,i,j} = -C_n \vec{V}_{i,j} \) is the normal damping force (N);
- \( \frac{dF_{ct,i,j}}{d\delta_i} = -K_t \) is the tangential force of contact (N), the value of which is limited by \( |F_{ct,i,j}| \leq \mu_s F_{cn,i,j} \);
- \( F_{dt,i,j} = -C_t \vec{V}_{i,j} \) is the tangential damping force (N);
- \( \vec{F}_{fl} \) is the drag force (N);
- \( \vec{T}_y = R \left( F_{ct,i,j} + F_{dt,i,j} \right) \) is the torque moment (Nm);
- \( \vec{M}_y = -\mu_t \left| F_{cn,i,j} \right| \frac{\vec{\omega}_i}{\left| \vec{\omega}_i \right|} \) is the friction torque (Nm);
- \( \vec{\Phi}_f \) is the drag moment (Nm);

\[
K_n = \frac{4}{3} E^* \sqrt{R^*}, \quad C_n = -\frac{\ln \varepsilon}{\sqrt{\pi^2 + (\ln \varepsilon)^2}}, \quad K_t = 2\sqrt{R \delta_i} \left( \frac{G_i}{2 - \nu_i} + \frac{G_j}{2 - \nu_j} \right), \quad C_t = K_s \sqrt{K_i/K_n}
\]

\( \delta_n \) and \( \delta_t \) are the normal and tangential contact displacement respectively:

\[
\frac{1}{E^*} = \frac{1 - \nu_i^2}{E_i} + \frac{1 - \nu_j^2}{E_j} \quad \text{and} \quad \frac{1}{R^*} = \frac{1}{|R_i|} + \frac{1}{|R_j|}
\]
where $E$ is Young’s modulus (Pa), $\nu$ is the Poisson ratio, $R_i$ is the particle radius (m), and $\mu_s$, $\mu_r$ are the sliding and rolling (m) friction coefficients respectively, and $\varepsilon$ is the restitution coefficient. The determination of interaction forces has been detailed by Lee et al. [15], Zhou et al. [16], and Nakashima [17].

5 EXPERIMENTAL PROCEDURE

The experimental shear tests were carried out in a 60.23 x 60.07 mm shear box (Figure 1). Samples made up of glass beads of uniform size were placed so as to have the maximum number of beads of glass per layer. However, because of the uniformity of the size of the glass beads, it is not always possible to fill the box so that there is no clearance between the rows of beads and the ends of the box. That is why, as we see in Figure 2, there is clearance between the glass bead row and the box (at the left-hand side and at the top). The size of this gap varies with the size of the beads, and it is distributed along the length and width of the sample during placement of the next row or when the load is applied. As a result, to facilitate the numerical modeling of the samples in the virtual laboratory, the glass beads have been placed so as to have the same number of glass beads per layer. Knowing the size of the glass beads and the length and width of the box, it is possible to determine the size of the gap between the rows of beads and the ends of the box, and thus simulate the arrangement of the glass beads during modeling. A special effort was made to ensure the appropriate placement of the glass beads in the shear box model. The glass bead diameter and the number of rows used for each size of glass bead are listed in Table 1. Table 2 presents the mechanical properties of the glass beads used.

![Figure 2: Photograph of the first layer of glass beads: (a) in the shear box; and (b) used for modeling](image)

Table 1: Glass bead diameter and number of rows

<table>
<thead>
<tr>
<th>Test</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass bead diameter (mm)</td>
<td>2.38125</td>
<td>3.175</td>
<td>3.96875</td>
<td>4.7625</td>
<td>6.35</td>
</tr>
<tr>
<td>Number of layers</td>
<td>8</td>
<td>6</td>
<td>5</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>
Table 2: Mechanical properties of the glass beads

<table>
<thead>
<tr>
<th>Mechanical properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus</td>
<td>62.784 GPa</td>
</tr>
<tr>
<td>Poisson Ratio</td>
<td>0.2</td>
</tr>
<tr>
<td>Density</td>
<td>2230 kg/m³</td>
</tr>
<tr>
<td>Coefficient of Restitution</td>
<td>0.87</td>
</tr>
<tr>
<td>Sliding Friction</td>
<td>0.02</td>
</tr>
<tr>
<td>Coefficient of Rolling Friction</td>
<td>5 × 10⁻⁵ m</td>
</tr>
</tbody>
</table>

6 PARALLELIZATION

Typically, numerical simulations using DEM are computationally intensive, either because they take a long time to complete or because they require access to substantial computing resources. In order to keep both simulation time and computational resource requirements to a minimum, the model was parallelized using GPU (Graphics Processing Units). Modern GPU are massive data parallel processors capable of handling over 500 billion operations per second, which makes them well suited to handling data bounded problems such as DEM simulations. Initial development was carried out on a 6 GB, 448 core Tesla M2070 GPU from Nvidia [18]. This particular card was chosen for its relatively large amount of memory, in order to reduce the amount of costly memory movement across the PCIe. For portability, we chose the OpenCL (Open Computing Language) framework [19], which offers an abstract view of the parallel architecture used. This allowed us to use both the CPU (Central Processing Units) and the GPU backend. OpenCL represent the data space as an n dimensional NDRange. This space is divided into work groups, which are then subdivided into fine grain work items. The Nvidia Fermi architecture divides compute cores among SM (Streaming Multiprocessors), which consist of blocks of 32 lock-stepped CUDA cores. Each particle interaction calculation was assigned to an OpenCL work item, which was then computed on an individual Cuda core.

7 VISUALIZATION

The visualization of large scale particle-to-particle interaction simulations poses multiple challenges. The sheer volume of data imposes either multiple static representations or a dynamic view, in order to permit observation of the entire system. In order to circumvent the problem of occluded particles, a dynamic 3D view of the model was chosen. Both classic 2D projection with transparency and the glass free autostereoscopic visualization approach were implemented. Using Alloscopy technology, we were able to project eight different perspectives on a screen covered by a lenticular array, resulting is seven simultaneously observable angles of vision. This technology allows multiple observers to interact with a simulation, and permits more complex systems to be viewed. The OpenGL (Open Graphics Library) API (Application Programming Interface) [20] was used to compute both the flat projection, as well as the different views required by the Alloscopy technology in a portable manner. GLSL (Graphics Library Shading Language) shaders were used to combine the
views into a single image projected on the screen, which is then redecomposed into individual images by the lenticular lens. OpenCL-OpenGL integration allows the reuse of particles from within the model without having to transfer data back to main memory.

The visualization plays an important role in the validation of numerical algorithms. It can help verify the correctness of the physical ideas used in the numerical modeling. It can also show paths that could not otherwise be considered, given the large datasets created during a computer simulation.

8 TEST RESULTS

A total of 20 shear tests were performed under vertical loads of 50 kPa, 160 kPa, 280 kPa, and 400 kPa on spherical glass beads of uniform size to validate the virtual laboratory results. In an attempt to verify the predictive capability of the DEM, closely matching 3D discrete element simulations of the shear tests were performed and compared with the experimental observations. Figures 3 to 7 show the results obtained, and the ability of the numerical simulation to capture the macroscopic response of the sample’s behaviour during the tests. However, the post peak response reveals differences, which can be attributed to the chaotic movement of the glass beads during testing.

These differences may be caused by one or more of the following uncertainties associated with the DEM hypothesis and with the experimental testing that are not accounted for in the model:

- The non sphericity of the glass beads that are assumed to be perfect spheres. The spheres used in the numerical modeling are perfect;
- The location of individual glass beads. To reproduce the exact location of every bead, a photograph of each layer was taken to reproduce that location precisely in the simulations. However, given that there is a clearance between the row of glass beads and the walls of the shear box, it is impossible to know the movement of every glass bead precisely when loads are applied;
- The small bead fragments resulting from breakage at the surface of the glass beads can influence their macroscopic behaviour. We can observe (Figure 8) the surface conditions before and after the tests;
- The large degree of uncertainty in the mechanical properties of the bead system;
- The contact formulation;
- The simulated particles are allowed to virtually overlap one another at contact points, as they are regarded as rigid bodies whereas in reality the particles deforms on contact;
- The main input parameters in the numerical model (i.e. normal and tangential stiffness, and a damping coefficient).

In terms of visualization possibilities, figure 9 shows four different shearing steps, and figure 10 depicts the intensity of the forces of contact between the particles.
**Figure 3:** Experimental and numerical results on samples made up of glass beads 2.38125 mm diameter

**Figure 4:** Experimental and numerical results on samples made up of glass beads 3.175 mm diameter

**Figure 5:** Experimental and numerical results on samples made up of glass beads 3.96875 mm diameter
Figure 6: Experimental and numerical results on samples made up of glass beads 4.7625 mm diameter

Figure 7: Experimental and numerical results on samples made up of glass beads 6.35 mm diameter

Figure 8: A closer view of a glass bead surface: (a) before and (b) after the shear tests
9 FUTURE WORK

A number of research projects are planned with the aim of developing our 3D Virtual Laboratory. Some of the topics of these projects are the following:

- Validation of the numerical results obtained by our 3D Virtual Laboratory for experimental shear tests carried out without clearance between the shear box and the glass beads;
- Validation of the numerical results obtained by our 3D Virtual Laboratory for various experimental tests on samples with the same grain size as they have in reality;
- Improvement of the capacity of our 3D Virtual Laboratory to understand the various phenomena encountered in the geotechnical field at the particle scale;
- Optimization of the various algorithms used in our 3D Virtual Laboratory, in order to reduce calculation times;
- Study of the sensitivity of the coefficients used in numerical simulations;
- Study of the effects of scale;
- Study of the influence on macroscopic behaviour of the water menisci between neighboring grains.

![Figure 9](image)

**Figure 9:** Example of the 3D visualization of four shearing steps (Glass bead diameter = 2.38125 mm)
10 CONCLUSION

The earlier work performed in our 3D Virtual Laboratory is presented in this paper. This laboratory was developed to meet needs encountered in the geotechnical field. The example presented in this article concerns only direct shear testing. The experimental and numerical results are in good agreement. Several factors explain the small differences, among them the locations of the glass beads during the trials and the inaccuracy of the coefficients used.

Our 3D Virtual Laboratory has the capacity to reproduce the shear tests on samples made up of glass beads, but also enables visualization of particle behaviour at macroscopic and particle level in 3D. This makes 3D simulation very practical from a quantitative standpoint.

REFERENCES


A DISCRETE ELEMENT APPROACH IN FRACTURE MECHANICS OF BRITTLE MATERIALS

BA DANH LE, GEORG KOVAL AND CYRILLE CHAZALLON

Laboratory of Engineering Design (LGECO)
National Institute of Applied Sciences of Strasbourg (INSA de Strasbourg)
24, Boulevard de la Victoire 67084 Strasbourg, France
e-mail: georg.koval@insa-strasbourg.fr

Key words: fracture mechanics, DEM, brittle materials

Abstract. In this study, we use the discrete element method (DEM) to model the fracture behavior of brittle materials in 2D. The material consists of a set of particles in contact with a close-packed structure. It allows us to derive an expression for the stress intensity factor as a function of the contact forces near the crack tip. A classical failure criterion, based on the material's toughness, is then adopted in the analysis of mixed mode crack propagation, represented by the contact loss between particles. We compare our model to classical solutions of tensile crack (mode I) and shear crack (mode II).

1 INTRODUCTION

The discrete element method (DEM) [1] is generally used in contact problems of a large number of particles. Material properties like elasticity, plasticity, viscosity, etc. can be modeled with different contact laws between particles. The introduction of bonded contacts with a limited resistance allow us to model brittle materials in fracture problems [2]. Although realistic macroscopic brittle behaviors are obtained with these models, a previous calibration of the contact laws is required [3].

Recent work of [4] presents analytical expressions which relate directly DEM material parameters to elastic continuous solid parameters (i.e. Young’s modulus and Poisson’s ratio). These expressions are based on a bidimensional close-packed assembly of particles. Considering this equivalence between discrete and continuous models in elasticity, we propose a DEM approach in fracture mechanics for brittle materials. The concordance with continuous classical theories exempt us of any previous calibration of the model parameters in order to attain convergent results.

This article begins with a presentation of the elastic contact law adopted in our simulations in Sec. 2. In Sec. 3, we present the theoretical elements of our discrete model in fracture mechanics. We compare our numerical results to classical cases of tensile and shear fracture in Sec. 4. Finally we present the conclusions of the work.
2 DEM IN ELASTICITY

Let us consider an homogenous (elastic and isotropic) material as an assembly of particles in contact. All mechanical properties of these particles are defined at the contact level (a local scale). The stresses are transmitted through contact forces, while material strain depends on particles translational and rotational motions.

2.1 Contact forces

We adopt a linear relation between contact forces and relative particle position which can be seen as a simplified version of Hertz contact model. Each force \( f_{ij} \) (applied by a particle \( j \) over a particle \( i \)) is decomposed in normal and tangential components. Let us define \( \vec{n}_{ij} \) as the normal vector pointing from the center of \( i \) to the center of \( j \) and \( \vec{t}_{ij} \) as the tangential vector, orthogonal to \( \vec{n}_{ij} \) and positively oriented (see Fig. 1).

The normal component is the sum of two contributions \( \vec{f}_{nij} = \vec{f}_{enij} + \vec{f}_{vinij} \). The elastic one, \( \vec{f}_{enij} = k_n \delta_n \vec{n}_{ij} \), depends on the normal deflection \( \delta_n \) and the normal stiffness \( k_n \). The inelastic one, \( \vec{f}_{vinij} = c_n \dot{\delta}_n \vec{n}_{ij} \) depends on a viscous damping parameter \( c_n \) and the time derivative of the normal deflection \( \dot{\delta}_n \). The latter contribution is only introduced to stabilize the numerical integration scheme. We choose \( c_n \) as a small fraction of \( \sqrt{mk_n} \) (where \( m \) is the particle mass) which guarantees a negligible inelastic effect.

The (elastic) tangential component \( \vec{t}_{ij} = k_t \delta_t \vec{t}_{ij} \) depends only on tangential relative displacement \( \delta_t \) and tangential stiffness \( k_t \).

![Contact model between two particles.](image)

2.2 Particle displacement and elastic behavior

The numerical approach is based on molecular dynamics method like in [1, 5]. The discrete particle motion equations are solved by Gear’s order three predictor-corrector algorithm [6].
A macroscopic strain tensor can be derived from particle displacements. The balance of the contact forces gives rise to a macroscopic stress tensor. Associating this equivalence between continuous and discrete approaches, [4] has shown that normal and tangential stiffness ($k_n$ and $k_t$, respectively) can be directly related to elasticity parameters of the continuous solid (Young’s modulus $E$ and Poisson’s ration $\nu$, for example).

3 DEM IN FRACTURE MECHANICS

In this section, we explore the similarity between discrete and continuous approaches in elasticity in order to derive expressions for the intensity factors in our discrete model. Based on these results, we deduce a crack propagation criterion for brittle materials in mixed mode.

3.1 Stress field near a crack tip

The singular stress field near a crack tip (in polar coordinates, see Fig. 2) can be written as in [7]:

\[
\sigma_{rr}(r, \theta) = \frac{K_{rr}(\theta)}{\sqrt{2\pi r}} \Rightarrow K_{rr}(\theta) = K_I \cos \frac{\theta}{2} \left(1 + \sin^2 \frac{\theta}{2}\right) + K_{II} \left(-\frac{5}{4} \sin \frac{\theta}{2} + \frac{3}{4} \sin \frac{3\theta}{2}\right),
\]

\[
\sigma_{\theta\theta}(r, \theta) = \frac{K_{\theta\theta}(\theta)}{\sqrt{2\pi r}} \Rightarrow K_{\theta\theta}(\theta) = K_I \cos \frac{\theta}{2} \left(1 - \sin^2 \frac{\theta}{2}\right) + K_{II} \left(-\frac{3}{4} \sin \frac{\theta}{2} - \frac{3}{4} \sin \frac{3\theta}{2}\right),
\]

and

\[
\sigma_{r\theta}(r, \theta) = \frac{K_{r\theta}(\theta)}{\sqrt{2\pi r}} \Rightarrow K_{r\theta}(\theta) = K_I \sin \frac{\theta}{2} \cos^2 \frac{\theta}{2} + K_{II} \left(\frac{1}{4} \cos \frac{\theta}{2} + \frac{3}{4} \cos \frac{3\theta}{2}\right),
\]

where $K_I$ and $K_{II}$ are the stress intensity factors [8]. $K_I$ is associated to opening mode, while $K_{II}$, to shear mode. Their values, which depend on loading and crack shape, quantify the strength of the singularity. For brittle materials they are directly associated to the energy release rate during crack extension [9].

**Figure 2:** Crack tip and singular stress field.
3.2 Mixed mode crack propagation - Maximum circumferential tensile stress

Presented by [10], this simple criterion for fracture propagation depends only on the knowledge of the stress state near the tip of a crack. This theory states that crack propagates in the plane perpendicular to the direction of greatest tension $\theta_0$ ($\sigma_{r\theta}(r, \theta_0) = 0$, or simply $K_{r\theta}(\theta_0) = 0$) when $K_{\theta\theta}(\theta_0) = K_{IC}$ (where $K_{IC}$ is the material toughness) [11].

3.3 Stress intensity factor $K_{\theta\theta}$ on the discrete approach

In our discrete approach, a crack may be represented by the absence of contact forces between some close particles, like the example in Fig. 3. The crack propagation is consequently modeled with the suppression of contact forces. So as to determine which contact should be suppressed, we seek the maximum value of $K_{\theta\theta}(\theta)$.

Let us consider a potential segment (composed by two consecutive contacts: $\textit{ik}$ and $\textit{jk}$) in a given direction $\theta$ next to a crack tip (see Fig. 4). Taking into account the contact forces acting over particles $\textit{i}$ and $\textit{j}$, the resultant force in $\theta$ direction is equal to:

$$ f'_\theta = \int n_{ik} \sin \alpha + \int t_{ik} \cos \alpha + \int n_{jk} \cos \alpha - \int t_{jk} \sin \alpha, $$

where $\int n$ and $\int t$ are normal and tangential contact forces respectively, and $\alpha = \pi/3$.

The resultant force $f_\theta$ might equilibrate the effect of $\sigma_{\theta\theta}$ (Eq. 1) along a straight distance $d$, where $d$ is the diameter of the particles (as can be seen in Fig. 4):

$$ f_\theta = \int_0^d \sigma_{\theta\theta} dr = \int_0^d \frac{K_{\theta\theta}(\theta)}{\sqrt{2\pi r}} dr = \sqrt{\frac{2d}{\pi}} K_{\theta\theta}(\theta). $$

The force $f'_\theta$ converges to $f_\theta$ for decreasing values of $d$. The comparison of Eqs. 2 and 3 leads to the approximation of the stress intensity factor $K_{\theta\theta}(\theta)$ as a function of contact forces in discrete approach.
Figure 4: Potential propagation segment in the discrete approach and corresponding contact forces.

Therefore a systematic analysis of all contact pairs allow the identification of the points that are susceptible to cracking. At a given segment, if the stress intensity $K_{\theta \theta}(\theta)$ reaches the material toughness value $K_{IC}$, the most tensioned contact (between $\vec{f}_{nik}$ and $\vec{f}_{njk}$) is suppressed and the crack propagates.

4 COMPARISON TO CLASSICAL RESULTS

In this section we compare our numerical results to classical solutions of fracture mechanics of brittle materials. Two situations are analyzed: pure tensile fracture (mode I) and pure (initial) shear fracture (mode II) in plane stress.

We suppose for simplicity that the particle diameter $d$ also corresponds to the thickness of the simulated bidimensional elements without loss of generality. The units of length and mass are respectively: $d$ and the particle mass $m$. This implies (for a given material toughness $K_{IC}$) $T = \sqrt{m/(K_{IC}\sqrt{d})}$ as time unit and $K_{IC}/\sqrt{d}$ as stress unit. Small strains are modeled taking $k_n = 10^4K_{IC}/\sqrt{d}$ as normal stiffness. The ratio between tangential and normal stiffness $k_t/k_n = 0.5$ (directly related to Poisson ratio) has no fundamental effect in plane stress results. We adopt a small value of viscous damping $c_n = 0.65\sqrt{mK_{IC}\sqrt{d}}$.

4.1 Tensile fracture

We present the results for two pre-cracked samples following the schemes presented in Fig. 5 (middle-crack tension panel) and Fig. 6 (double edge notch tension panel). A
vertical displacement induces a mean tensile stress $\sigma$ to the sample. We measure the maximum stress value $\sigma_{\text{max}}$ supported by the structure before complete fracture. The panels have a rectangular shape with height equal to 3 times width to avoid eventual boundary effects.

\section*{Figure 5: Tensile test - middle-crack panel.}

\section*{Figure 6: Tensile test - double edge notch panel.}

Our numerical results of $\sigma_{\text{max}}$ are compared to the following expressions [7]:

- middle-crack tension panel

$$\sigma_{\text{max}} = \frac{K_{\text{IC}}}{\sqrt{\pi a}} \left[ 1 + 0.256(a/L) - 1.152(a/L)^{2} + 12.22(a/L)^{3} \right]^{-1},$$

(5)
double edge notch tension panel

$$\sigma_{\text{max}} = \frac{K_{IC}}{\sqrt{\pi a}} \left[ 1.12 + 0.43(a/L) - 4.79(a/L)^2 + 15.46(a/L)^3 \right]^{-1}. \quad (6)$$

In both cases, four different crack lengths $a/L$ were tested: $3/22, 4/22, 5/22, \text{ and } 6/22$. The maximum stress $\sigma_{\text{max}}$ supported by the panels before fracture propagation decreases when crack length grows as shown in Fig. 7. The systematic variation of the ratio $L/d$ allows the analysis of the discrete approach convergence. Higher values of $L/d$ are associated to more precise descriptions of the crack zone inducing better results whatever the crack type.

Figure 7: Normalized maximum stress $\sigma_{\text{max}}\sqrt{L}/K_{IC}$ as a function of the crack length $a/L$ for the (a) middle-crack and (b) double edge notch panels.

In order to verify any eventual effect of the particle disposition on the results, we have also tested samples with an orthogonal orientation (compared to Fig. 3). A similar convergence (compared to Fig. 7) indicates the generality of the Eq. 4 with respect to the direction.

4.2 Shear fracture

Shear stress may induce crack branching under certain conditions. Let us consider a square plate (side length $L$) under biaxial stresses (lateral compression $\sigma_x$ and vertical tension $\sigma_y$) with an initial inclined crack of length $a$ (see Fig. 8). Depending on the initial crack angle $\alpha$, a pure shear stress condition (in $\alpha$ direction) can be obtained if $\sigma_x/\sigma_y = \tan^2 \alpha$. Following the maximum circumferential tensile stress criterion (Sec. 3.2), for pure shear stress ($K_I = 0$), the angle which maximizes $\sigma_{\theta\theta}$ (Eq. 1) is $\theta_0 = 70.5^\circ$ (relative to $\alpha$). The crack branching angle $\theta_0$ is only a prediction of the initial crack propagation. The general tendency of the crack is to become horizontal, orthogonal to stress tensile direction.
The results of the simulation of an inclined crack with $\alpha = 60^o$, $a/L = 0.41$, $L/d = 176$ are shown in Fig. 9. The crack propagation presents a coherent path tending slightly to an horizontal direction (see Fig. 9a). In detail, at Fig. 9b, the theoretical prediction of the initial crack branching is fairly obtained.

![Figure 8: Square plate with an inclined crack under biaxial loading. The dotted lines indicate the crack propagation path.](image)

5 CONCLUSIONS

We propose in this article DEM approach in fracture mechanics of isotropic brittle materials entirely compatible with continuous classical theory. Based on the equivalence
between discrete and continuous approaches in elasticity, we present an expression for the stress intensity factor $K_{\theta\theta}$ (in polar coordinates) as a function of the forces of two adjacent contacts. The well known "maximum circumferential tensile stress” criterion for mixed mode crack propagation is then associated to allow the study of complex plane cracks. The toughness of the material is directly introduced as a model parameter without any previous calibration, which represents an important feature.

The simplicity of the formulation is followed by encouraging numerical results. The DEM approach is compared to two tensile cases (mode I); both presenting a monotone convergence towards classical solutions for more precise discretization (evaluated by the ratio $L/d$). The effect of shear stresses (mode II) is analyzed through a biaxial test of a sample with an initial inclined crack. The initial crack branching follows the theoretical prediction as well as the general evolution of the crack.

As perspective, we consider the study of interfacial cracks (between different materials) and the effect of compression loading (with crack closure). Both cases can easily be implemented for multiple cracks with DEM methods.

REFERENCES


A STUDY ON THE INFLUENCE OF THE PARTICLE PACKING FRACTION ON THE PERFORMANCE OF A MULTILEVEL CONTACT DETECTION ALGORITHM

V. OGARKO AND S. LUDING

Multi Scale Mechanics (MSM), CTW, UTwente,
PO Box 217, 7500 AE Enschede, Netherlands;
v.ogarko@utwente.nl, s.luding@utwente.nl

Key words: contact detection, discrete element, polydisperse, particle size distribution, packing fraction

Abstract. We investigate the influence of the packing fraction of highly polydisperse particle systems on the performance of a high-performance multilevel contact detection algorithm as applied for molecular dynamics type simulations. For best performance, this algorithm requires two or more hierarchy levels in order to cope with the strongly different particle size classes. In order to predict the optimal number of levels, an empirical parameter corresponding to the “overhead” is identified. For homogeneous systems, the density is not much affecting the performance of the algorithm, however, the optimal number of levels slightly increases with density as well as the speed-up as compared to a single-level method.

1 INTRODUCTION

Contact detection is a fundamental computational problem arising in computer simulations of systems consisting of many discrete objects such as particles or atoms. The particle based modeling methods like the Discrete Element Method (DEM) [1] play an important role for physics-based simulations in many diverse fields. The performance of the computation relies on several factors, which include the physical model, on the one hand, and the contact detection method used, on the other. The collision detection of short-range pairwise interactions between particles is usually one of the most time-consuming tasks in calculations [2].

The most commonly used method for contact detection of nearly monosized particles with short-ranged forces is the Linked-Cell method [3]. Nevertheless, the Linked-Cell method is unable to efficiently deal with particles of greatly varying sizes [4]. This can effectively be addressed by the use of methods based on hierarchical grids [4, 5, 6].
The multilevel contact detection algorithm presented in Ref. [6] contains the number of hierarchy levels and the cell sizes at each level as adjustable parameters. A method to find the optimal parameters for an arbitrary polydisperse size distribution of objects is also shown in [6]. As an input parameter, this method requires the “overhead” of the data structure. In addition to the detailed study of different size distributions in Ref. [6], we examine the influence of the density of the particle system on the performance of the algorithm [6] and on the “overhead” of the data structure by means of molecular dynamics simulations.

2 CONTACT DETECTION ALGORITHM

In this section we briefly describe the main ideas of the multilevel contact detection algorithm and the method to find the optimal parameters, which are necessary for understanding the results of this study. For more details see Ref. [6].

2.1 Algorithm

The algorithm is designed to determine all the pairs in a set of \( N \) spherical particles in a \( d \)-dimensional Euclidean space that are in close neighborhood and possibly do overlap. A hierarchical grid structure used in the algorithm is a set of \( L \) regular grids with different cell sizes. Every regular grid is associated with a hierarchy level \( h \in [1, L] \), where \( L \) is the integer number of hierarchy levels. Each level \( h \) has a different cell size \( s_h \in \mathbb{R} \), where the cells are \( d \)-dimensional cubes. Grids are ordered with increasing cell size so that \( h = 1 \) corresponds to the grid with smallest cell size, i.e. \( s_h < s_{h+1} \). For a given number of levels and cell sizes, the hierarchical grid cells are defined by the following spatial mapping of points \( \vec{x} \in \mathbb{R}^d \) to a cell at specified level \( h \):

\[
(\vec{x}, h) \mapsto ([x_1/s_h], ..., [x_d/s_h], h),
\]

(1)

where \( [x] \) denotes the floor function \(^1\).

The algorithm is made up of two phases. In the first “mapping phase” all the particles are mapped into hierarchical grid cells based on their location and size as follows. The diameter of the smallest particle within a given level of hierarchy should be larger than the cell size of the previous level of hierarchy, and the diameter of the largest particle at some hierarchical level should be smaller or equal to the cell size of this level. The cell-sizes and the distribution of particles among levels are detailed below.

In the second “contact detection phase” for every particle in the system the potential contact partners are determined, and the geometrical intersection tests with them are made. The contact detection is split into two steps, and the search is done by looping over all particles and performing the first and second steps consecutively for each particle. The first step is the contact search at the level of insertion of a given particle, using the classical Linked-Cell method [3]. The second step is the cross-level search. For a

\(^1\)The largest integer not greater than \( x \)
given particle, one searches for potential contacts at every level $h$ lower than the level of insertion. For detailed description of these steps and further optimizations see Ref. [6].

2.2 Optimal parameters

It is shown in Ref. [6] that in the case of polydisperse systems, i.e., systems where all the particles’ sizes are different, the performance of the multilevel contact detection algorithm strongly depends on the selected parameters (the number of levels $L$ and cell sizes $s_h$). Furthermore, a hypothesis on the optimal distribution of particles by levels was formulated in [6], which states:

**Hypothesis 1** Let $m_h$ be the average number of particles per cell at level $h$, that is, $m_h = N_h/N_c^h$, where $N_h$ is the number of particles at level $h$, and $N_c^h$ is the number of cells at this level. Then the optimal distribution of particles by levels satisfies the following condition:

$$m := m_i = m_j, \text{ for all } i, j \in [1, L].$$

If the particles are mapped to the levels, such that Eq. (2) is approximated, the CPU time spent for contact detection, $T_{CD}$, scales as

$$T_{CD} \sim NL(m + K),$$

where $K$ is a constant corresponding to the “overhead” of the algorithm, i.e., the time spent to access cells to be tested, and $m = m(L, PSD)$ is the number of particles per cell (see Ref. [6]). To compute $m$ for a given $L$ and for the particle system at hand, one needs to choose cell sizes $s_h$ so that Eq. (2) is approximately satisfied. How to do this is explained in Ref. [6]. In the next section we investigate the influence of the volume fraction of the particle system, i.e., the ratio between the volume of the particles and the volume of the system, on the value of the “overhead” $K$.

3 SIMULATION RESULTS

We use homogeneous and isotropic disordered systems of colliding elastic spherical particles in a cubical box with hard walls. The motion of particles is governed by Newton’s second law with a linear elastic contact force during overlap. Every particle undergoes only translational motion (without rotation) and gravity is set to zero.

3.1 Experimental setup

The systems are prepared in two stages. Starting from a random uniform distribution of points in a cubical box, the radius of the particles grows linearly with time. We use non-overlapping spheres [7], with an Event-Driven code [8], whose growing rate conforms to and conserves a prescribed size distribution. Initial velocities are set randomly in order to keep the system dynamic and random, for details see Ref. [8]. When the target volume fraction is reached, the growth process is stopped.
Figure 1: Particle systems with $N = 125001$ with (a) volume fraction $\nu = 0.1$, (b) volume fraction $\nu = 0.4$, with uniform volume distribution. The size ratio $\omega$ is 50. Colour is by relative size.

With the final configuration from the first step, the simulation switches to the relaxation stage with “soft” particles, i.e., particles move according to interparticle forces [1]. The linear elastic normal contact force model is used [9], which leads to a certain contact duration. At the beginning of this stage the velocities of the particles are scaled in a way that a collision between two of the smallest particles would reach an average maximum overlap of one percent of their radius. We let the simulations run for a few collisions per particle for equilibration before making the measurement of the performance, in order to have contacts (overlaps) between particles in the system.

We use uniform volume size distribution, i.e., the probability distribution of the volumes of the particles is constant. This type of size distribution implies that the particle system contains rather many small particles. We denote the size ratio between the radius of the largest and the smallest particle in the system as $\omega$.

3.2 Numerical performance results

We measure the total CPU time for varying number of hierarchy levels $L$ for particle systems with different volume fractions. For this, we calculate the value of $m$ for each $L \in [1, 50]$ using the method given in Ref. [6], and run simulations where the multilevel grid is used with $L$ levels, and the cell sizes $s_k$ are computed in accordance with hypothesis (1). To present the total CPU time, we use the slowdown factor $SF$, that is the total CPU time divided by the smallest CPU time for a given system. In Fig. 2 the results of this numerical experiment are shown for systems with uniform volume distribution, with $N = 125001$ and $\omega = 50$. The analytical prediction (3) is also plotted with $K = 0.2$,.
scaled in such a way that $SF = 1$ corresponds to the minimum of the right hand side of Eq. (3). Note that even though the prediction (3) is for CPU time spent only for contact detection, $T_{CD}$, the total CPU time for fixed number of particles also scales as $T_{CD}$. This is because the CPU time spent in the force calculation and integration does not depend on the grid parameters used. From the numerical experimental results shown in Fig. 2 it can be seen that the prediction of Eq. (3) used with $K = 0.2$ can be used for determining the optimum number of levels, and the value of $K$ is not dependent on the packing fraction. We also confirm that the dependence on density is very weak for rather large packing fractions of 0.62 (data from Ref. [6] – not shown here). Furthermore, the optimal number of levels, $L^*$, slightly increases with the volume fraction from $L^* = 5$ for $\nu = 0.1$ to $L^* = 8$ for $\nu = 0.62$, see Fig. 3(a). Finally, the best speed-up over the Linked-Cell method ($L = 1$), $S$, increases nearly linearly with the volume fraction, as it can be seen from Fig. 3(b). Note that even for relatively low volume fraction $\nu = 0.1$, the speed-up is high, i.e., $S \approx 150$, so the use of the multilevel algorithm is highly advantageous for this type of particle size distributions (many small particles) for the whole range of volume fractions.

Figure 2: Slowdown factor for different numbers of levels for systems with $N = 125001$ and $\omega = 50$ with uniform volume distribution; (a) volume fraction $\nu = 0.1$, (b) volume fraction $\nu = 0.4$. The prediction of Eq. (3) is used with $K = 0.2$ for plotting solid lines. Note that the data can be obtained only for integer values of $L$. 

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4 SUMMARY AND CONCLUSIONS

We have shown that the multilevel algorithm presented in Ref. [6] can be used to significantly improve the performance of simulations of particle systems with rather many small particles at very different volume fractions. The speed-up relative to the single-level Linked-Cell method increases nearly linearly with the volume fraction for the homogeneous systems tested. Moreover, the value of the “overhead” parameter, which is necessary to analytically find the optimal number of hierarchy levels is not dependent on the packing fraction for these systems. This leads to an increasing number of levels with the density for optimal performance of the contact detection.

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COUPLED LATTICE BOLTZMANN – DISCRETE ELEMENT METHOD FOR NUMERICAL MODELLING OF SAND PRODUCTION

ALI GHAASSEMI* AND ALI PAK†

* Faculty of Architecture and Civil Engineering
Islamic Azad University, Qazvin Branch
Qazvin, Iran
e-mail: a_ghassemi@qiau.ac.ir, www.qiau.ac.ir

† Civil Engineering Department
Sharif University of Technology
Tehran, Iran
e-mail: pak@sharif.edu, www.sharif.edu

Key words: Sand Production, Lattice Boltzmann Method, Discrete Element Method.

Abstract. In this study, a coupled numerical approach based on Lattice Boltzmann Method (LBM) and Discrete Element Method (DEM) is employed for 2D simulation of fluid flow in porous media comprising of movable circular particles. The developed model is used for simulation of sand production which is one of the important problems in petroleum industry. The numerical tool has proved to have the capability of investigating the mechanisms involved in sand production problem. The results show that the rate of sand production is strongly affected by flow rate and confining pressure.

1 INTRODUCTION

A common challenge in hydrocarbon extraction from sandstone reservoirs is sand production. Production of sand particles during the oil recovery process initiates when stress changes imposed by fluid flow causes shear failure in weakly or unconsolidated rock mass near the well. It is followed by transportation of dislocated sand particles into the production well which adversely affects the well stability and disturb the pipelines and equipment. High rate of sanding may finally lead to massive sand production which blocks the well casing perforations and break the oil production. However, it has been proven that limited sand production may significantly increase the well [1].

Many researchers have attempted modelling of sand production problem through using theoretical or numerical approaches. Strong non-linear processes involved in sand production such as high changes in compressibility of rock matrix and permeability of sandstone increase the complexity of numerical simulation of this coupled hydro-mechanical phenomenon [2]. A review of modelling strategies can be found in [3].

In this paper, a newly developed numerical model has been employed to study the mechanisms influencing sand production at pore scale. Using the Discrete Element Method and the Lattice Boltzmann Method in a coupled manner, the numerical model can simulate the tortuous flow of fluid in deformable particulate media as well as capturing the destabilization
of sand arches around a perforation and the erosion process of the failed sand grains.

2 PORE SCALE MECHANICS OF SAND PRODUCTION

Sand production is resultant of a series of micro-scale processes that occur near the casing perforations. The flow of fluid through pore spaces of rock mass imposes drag forces on the individual sand grains. The fluid properties such as viscosity and density have direct effects on the magnitude of the induced drag forces. As the hydraulic gradient of the flow is much higher near wellbore zones, the tortuous velocity of flowing fluid increases greatly, which as a result, causes higher drag forces on solid grains adjacent to the perforations. For weakly cemented sandstone, where enough cohesion resistance is not available, if the drag forces overcome the friction and interlocking between particles, sand grains may dislodge from the mass and become displaced by flowing fluid. This erosion of solid particles from porous medium makes larger canals for fluid flow and consequently increases the flux of both fluid and the produced sand particles. During the above process, sand arching may occur at the perforations near the wellbore. Forming of arches can significantly reduce the amount of produced solids. However, stability of arches is highly dependent on perforation size, particle size distribution and stress level.

Therefore, theorization of sand production problem seeks for understanding the pore scale hydro-mechanical events which dominate the behavior of the system. Despite this fact, linkages between micro-structural deformation mechanisms and observed sanding rates have not been established yet [4]. In this study, it is endeavored to investigate the role of pore scale mechanisms that are responsible for sand production.

3 COUPLED LB-DE MODEL

3.1 Background

Traditional continuum-based models such as Finite Element Method (FEM) are typically not adequate for capturing such local discontinuous behavior [3]. On the other hand, numerical models such as Discrete Element Method (DEM) in which sand grains are represented by distinct elements and their interaction can be simulated explicitly are very favorable for modeling sand production. The work of O’Connor et al. [5] is the one of the first efforts to examine the ability of DEM to model the mechanics of sand production. Dorfmann et al. [6] utilized a DEM model to simulate the sand production and arching effects around a cavity. In their study, capillary forces between adjacent grains were included in the DEM model to compare the effect of pressure gradient and capillary forces on the formation of stable arch configuration around a cavity. Jensen et al. [7] modeled sand production using the coupling of two dimensional DEM and finite element implementation of the two-dimensional continuity equation for Darcy flow. Their simulation shows that as the strength of the cohesive bonds decreases, the number of particles breaking free from the matrix increases.

To represent fluid–solid interaction at the local scale, it is more delicate to simulate the fluid flow in the pore space at a resolution finer than that of pores and grains [8]. Among a number of microscopic numerical methods in the context of computational fluid dynamics, Lattice Boltzmann Method (LBM) has proven to be a versatile method for simulation of fluid flow in systems with complex solid boundary conditions such as porous media. The particle-
like nature of LBM permits a transparent handling of irregular flow paths through particulate media using elementary mechanical events such as mirror and bounce-back reflections without comprising great computational costs. Coupled LB-DE model was first introduced by Cook [9]. In the coupling scheme, the velocity of the fluid adjacent to solid surfaces is set to velocity of solid to retain the no-slip boundary condition. The two-dimensional LB-DE model has been validated through a number of benchmark problems including Coutte flow, particle sedimentation and drafting-kissing-tumbling phenomenon [9, 10]. Recently, the coupled LB-DE model was applied for modeling simplified forms of some engineering issues such as sand boiling in granular soils [11], vacuum dredging [12] and sand production [4].

3.2 Theoretical aspects of coupled LB-DE model

Discrete Element Method

Discrete element method (DEM has become a powerful numerical tool for analyzing particulate media since it was first introduced by Cundall & Strack [13]. The discrete element method conceives granular materials as an assemblage of distinct rigid particles. Solid rigid particles can interact among each other or with solid boundaries when overlap of boundaries occurs between particle/particle or particle/wall. By using the contact-force displacement law, the forces at contacts are related to the magnitude of the overlaps. The displacement and velocity of each individual solid particle are calculated from the summation of all forces acting on the particle using Newton’s second law of motion. This calculation cycle is performed in each time step during the analysis.

The force-displacement law establishes a relationship between the contact force and the magnitude of particle overlap by the following equations:

$$\Delta F_n = K_n \Delta \rho_n; \quad \Delta F_t = K_t \Delta \rho_t$$

where $\Delta F$, $K$, and $\Delta$ are incremental force, stiffness, and magnitude of particle overlap, respectively. The subscripts $n$ and $t$ represent normal and tangential directions with respect to the plane of particle overlap. Then, contact forces between each two contacting particles are updated:

$$F_{i,n}^{t+1} = F_{i,n}^{t} + \Delta F_{n} \quad , \quad F_{i,t}^{t+1} = F_{i,t}^{t} + \Delta F_{t}$$

(2)

The tangential contact forces are usually governed by some frictional relationships. The Coulomb criterion was adopted in this study. Accordingly, the commencement of slippage occurs where the tangential contact force exceeds the following criterion:

$$F_{c,j}^{t,\max} = \mu_s F_{c,j}^{t,n} + c$$

(3)

where $\mu_s$ is the sliding friction coefficient between two contacting solid particles and $F_{c,j}^{t,n}$ and $F_{c,j}^{t,t}$ are the normal and tangential contact forces on particle $j$.

Newton’s second law of motion describes the relationship between the acting forces and the movement of particles. The 2D form of this law which has been applied in the developed DEM code for current study is given by:
\[ m_j \ddot{x}_j = \sum F_j \]  
\[ I_j \ddot{\theta}_j = \sum M_j \]  

(4) \hspace{2cm} (5)

where \( \ddot{x}_{i,j} \) and \( \ddot{\theta}_j \) are linear and angular accelerations of particle \( j \) at direction \( i \) and \( m_j \) and \( I_j \) are the mass and moment of inertia of discrete particle \( j \), respectively.

A few models have been proposed for incorporating the rolling resistance in DEM, which can be classified into two categories: angular-velocity-dependent and -independent, as have been discussed by Zhu & Yu [14]. Herein, the angular-velocity independent model was chosen because it is simpler and more effective.

Based on the modified algorithm, Equation (5) can be rewritten as follows:

\[ I_j \ddot{\theta}_j = \sum \left[ \left(F_{c,j} \times \mathbb{R}_j\right) - \mu_r R_j \mathbb{F}_{c,j} \mathbb{R}_j + M_{nc,j} \right], \quad \lambda = \text{sign} (F_{c,j}) \]  

(6)

where \( \mathbb{R}_j \) is the radius of particle \( j \), \( \mu_r \) is the rolling friction coefficient and \( M_{nc,j} \) is the part of moment on particle \( j \) which is induced by non-contact forces. \( \mu_r \) is a dimensionless parameter which is dominated by roundness of contacting particles.

### Lattice Boltzmann Method

Unlike the traditional CFD methods that directly solve the Navier-Stokes equations, LBM actually simulates macroscopic flows by means of a particulate approach. LBM was applied to porous flow soon after its emergence in 1989 [15]. Later studies confirmed the reliability of LBM in modeling flow through porous media (e.g. Pan et al. [16] and Ghassemi & Pak [17]).

In LBM, the spatial space is discretized in a way that it is consistent with the kinetic equation. In this method, space is divided into regular lattices with the same spacing \( h \) in both x- and y-directions and at each lattice site a particle distribution function \( f_m(x,t) \) is defined which is equal to the expected number of identical fluid particles at that site \( x \) in the direction of \( m \). During each discrete time step of the simulation \( (\Delta t_{LB}) \), fluid particles move to the nearest lattice site along their direction of motion with different velocities of \( \bar{v}_m \), where they “collide” with other bundles of fluid particles that arrive at the same site. The outcome of the collision is determined by solving the Boltzmann equation for the new particle distribution function at that site and the particle distribution function is updated. The magnitude of speed in different directions which is called lattice speed is defined as \( C = h/\Delta t_{LB} \).

Propagation and collision of fluid particles in LBM can be mathematically summarized by the below two-step scheme, respectively:

\[ f_m (x + \bar{v}_m \Delta t, t + \Delta t) = f_m (x, t) \]  
\[ f_m^{\text{updated}} (x, t) = \Omega_m (f (x, t)) \]  

(7) \hspace{2cm} (8)

The collision rule \( \Omega \) should be chosen to leave the sum of the \( f_m (x, t) \) unchanged (no fluid particles are lost.) The rule is also selected to conserve the total momentum at each lattice site.
The single relaxation time BGK (after Bhatnagar, Gross, and Krook [18]) operator approach is an uncomplicated approach which simply approximates the collision by assuming that the momenta of the interacting fluid particles will be redistributed at some constant rate toward an equilibrium distribution \( f_m^{\text{eq}} \). BGK allows one to solve the equilibrium distribution such that the microscopic equations are satisfied and the Navier-Stokes equations are recovered. In BGK lattice Boltzmann method, collision rule is given by:

\[
\Omega_m (x,t) = f_m (x,t) - \frac{\Delta t_{\text{LB}}}{\lambda} (f_m (x,t) - f_m^{\text{eq}} (x,t))
\]

where \( f_m^{\text{eq}} \) is the local equilibrium density distribution for the fluid and \( \lambda \) is relaxation parameter. The two-dimensional model implemented in this study uses a square, nine-velocity lattice typically referred to as D2Q9 model. For this model, \( f_m^{\text{eq}} \) is given by [19]:

\[
f_0^{\text{eq}} = w_0 \rho (1 - \frac{3}{2} \mathbf{V} \cdot \mathbf{V})
\]

\[
f_m^{\text{eq}} = w_m \rho \left[ 1 + \frac{3}{C^2} (\mathbf{e}_m \cdot \mathbf{V}) + \frac{9}{2C^2} (\mathbf{e}_m \cdot \mathbf{V})^2 - \frac{3}{2C^2} (\mathbf{V} \cdot \mathbf{V}) \right], \quad m = 1, 2, ..., 8
\]

in which \( \rho \) and \( \mathbf{V} \) are macroscopic fluid density and velocity and \( w_m \) are the fixed weighting values: \( w_0 = \frac{4}{9}, \ w_{1,2,3,4} = \frac{1}{9}, \ w_{5,6,7,8} = \frac{1}{36} \).

The macroscopic parameters are regained by:

\[
\rho = \sum_{m=0}^{8} f_m, \quad \rho \mathbf{V} = \sum_{m=1}^{8} f_m \mathbf{v}_m
\]

The dimensionless relaxation parameter \( \tau = \frac{\lambda}{\Delta t_{\text{LB}}} \) is related to the fluid viscosity by:

\[
\nu = \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{h^2}{\Delta t_{\text{LB}}}
\]

**Coupling approach**

In this study, a weakly coupling scheme similar to what has been used by Cook [9] is employed. During each time step, the LB code is called to simulate the fluid flow and the hydrodynamic forces and moments on individual particles are calculated and then exported to DEM as input data. In DEM, the fluid-induced forces are combined with other existing forces acting on particles to determine the new position of particles. Since the time step for LB in our simulations is always greater than the time step for DE, each LB calculation cycle is accompanied with a number of DEM calculation cycles during which the hydrodynamic forces are unchanged.

Different methods are available in LB literature for obtaining hydrodynamic forces acting on the particles moving on the LB lattice [20, 21 and 22]. Herein, the immersed moving boundary method [21] was employed since it has been successfully applied and verified by majority of previous researches on DE-LB simulations [9, 10, 23]. In this method, the collision rule (Equation (9)) is modified to incorporate the influence of the solid particles:
\[ f_i(x + e \Delta t, t + \Delta t) = f_i(x, t) - \frac{1}{\tau} [1 - B][f_i(x, t) - f_i^{eq}] + Bf_i^n \tag{14} \]

For each lattice node, weighting parameter \( B \) is defined as a function of solid ratio which is the ratio of area occupied by solid to the total area of the \( h \times h \) computational cell around the lattice node [23]. \( f_i^n \) is an additional collision term that bounces back the non-equilibrium part of the distribution which is given by Cook [9] as:

\[ f_i^n = f_i^{eq}(\rho, v_s) - f_i^{eq}(\rho, v_s) + f_i(x, t) - f_i(x, t) \tag{15} \]

where \( v_s \) is the velocity of the solid and the subscript \(-i\) indicates the direction opposite to \( i \). According to this approach, the fluid induced hydrodynamic force and torque on a solid particle mapped on \( n \) lattice nodes is calculated by the following equations, respectively:

\[ F = Ch \left[ \sum_k (B_k \sum_i f_i^n e_i) \right] \tag{16} \]

\[ T = Ch \left[ \sum_u (x_k - x_u) \times (B_u \sum_i f_i^n e_i) \right] \tag{17} \]

where \( x_k \) and \( x_u \) are the coordination of node \( k \) and center of particle, respectively.

2D LB modeling of fluid flow through compacted particulate samples in which solid particles are in physical contact with neighboring particles may not be efficient because there may be inadequate interconnected pores to allow the fluid particles to flow through the 2D system. This problem can be solved numerically by using hydraulic radius multiplier technique. In this approach, the mechanical radius of particles is reduced in LB simulations to resolve the flow of the fluid through the sample [4]. The hydraulic radius is only considered for LB code and the real (mechanical) radius is still used in DE calculations.

Verification of the developed coupled LB-DE code has been discussed elsewhere [24].

4 NUMERICAL MODELING OF SAND PACK EXPERIMENT

4.1 Sand pack experiment

In the present study, a series of sand pack experiments conducted by Al-Awad et al. [25] was considered for numerical simulation by the developed model. In sand pack tests, a viscous fluid permeates through a confined cylindrical sand sample at one end, thereby inducing sand production at the other end through a small orifice. In their work, sand packs were constructed analogous to samples obtained from certain reservoir and they studied the amount of sand production under different conditions of flow rate and confining pressure. The sand packs had an inside diameter of 3.81 cm and 8 cm length and the diameter of the orifice is 4 mm. The porosity of all constructed samples was about 0.45.

4.2 Numerical simulation

Numerical modeling of the whole sand pack is not currently possible because of high
computational costs. Therefore, only part of sample near the outlet of sand box was considered for numerical simulation as depicted on Figure 1. Thus, the model may not be able to simulate the complete sand production cycle in which production of sand stops after development of a stable cavity especially for higher flow rates. Despite this shortcoming, the numerical model is capable of predicting the onset of sanding and rate of sand production at early time of production.

The sand sample for numerical simulations was created by particle packing technique using DEM [17]. The porosity of the created sample was about 0.16 and the grain size distribution of the sample is shown in Table 1. Because of 2D nature of the model, this porosity cannot directly be compared with that of the real sample. In turn, porosity of the model can be adjusted by changing the hydraulic radius multiplier (sec. 3-2) in a manner that the intrinsic permeability of the sample is equivalent to that of real porous medium.

For coupled analyses, a difference in fluid pressure was applied at two opposite sides of the soil sample in order to induce the flow towards the outlet, and the other two sides are treated as no-slip boundaries. Discretization of the domain needs to be fine enough in order to adequately resolve the fluid flow in the numerous small pores created by the finest solid particles, and also to provide adequate resolution for smooth variations of hydrodynamic forces when solid particles are moving on the fluid lattice. In this work, lattice spacing varied between 0.012 to 0.018 mm in different analyses. The values of other LB parameters used in this study are listed in Table 2.

![Laboratory Sand Pack](image)

**Figure 1**: Dimensions of laboratory sand pack and simulation domain

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of particles</td>
<td>7500</td>
</tr>
<tr>
<td>D (mm) [weight percentage %]</td>
<td>0.6 [2], 0.3 [43], 0.25 [20], 0.125 [35]</td>
</tr>
<tr>
<td>ρs (kg/m³)</td>
<td>2600</td>
</tr>
<tr>
<td>Kn , Ks (N/m)</td>
<td>10¹</td>
</tr>
<tr>
<td>μs , μr</td>
<td>1.0, 0.2</td>
</tr>
</tbody>
</table>

**Table 1**: DEM parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>h (mm)</td>
<td>0.018, 0.014, 0.012</td>
</tr>
<tr>
<td>r</td>
<td>0.52</td>
</tr>
<tr>
<td>ν (m²/s)</td>
<td>1.05×10⁻⁷</td>
</tr>
</tbody>
</table>

**Table 2**: LBM parameters
The main DEM parameters used for simulation of sand erosion is gathered in Table 1. High values of friction coefficients were chosen to compensate for the low shear strength of the assembly of circular disks comparing to the real sand pack which contains grains with irregular shapes. However, early numerical results showed that a small value for interparticle cohesion is also required to artificially simulate the absence of interlocking resistance between circular particles in the numerical model. Constant stress boundary condition was applied for the top, bottom, and left walls using a servo-control approach in which the walls are allowed to displace in order to retain the required constant stress level on the walls.

5 RESULTS AND DISCUSSIONS

Prevailing failure mechanism for sand production depends on the values of in situ effective stresses and flow rate in relation to rock strength [26]. For weak sandstone, sand is produced when drag forces caused by flowing fluid exceed the formation strength which is mainly supplied by true cohesion of natural cementing materials, resistance developed by inter-particle friction controlled by normal contact forces, and the apparent cohesion induced by interlocking between sand grains. For unconsolidated rock mass, the true cohesion is not available and rock resistance against erosion of sand grains by fluid induced forces (tensile failure) can only be attributed to inter-particle forces and interlocking between sand grains.

From the above discussion, for condition of the sand pack experiment considered for numerical simulation in this study (where no cementing material exist in the sample), the level of drag forces induced by fluid flow as well as inter-particle forces governed by applied confining pressure around the sample are the most important factors influencing the sanding initiation through the small perforation. In the following sections, the results of numerical analyses for different conditions of flow rates and confining pressures are discussed.

5.1 Effect of flow rate

The results of some of the analyses in terms of cumulative weight of the produced sand versus time for two different applied pressure gradients are shown in Figure 2. The quantity of the produced sand has been calculated from the number of solid grains passing the orifice. Initial high rate of sand production at the early times of simulation (before 0.05 s) for both cases is due to the exit of sand particles in the vicinity of the orifice immediate after removing the wall. However, for lower pressure gradient ($\nabla p = 0.10 \text{ MPA/m}$), formation of stable cavity around the perforation caused stopping the sand production, for higher pressure gradient ($\nabla p = 0.44 \text{ MPA/m}$) sand production continues up to end of the simulations. The variation of flow rate with time was also plotted on the figures. For lower pressure gradient (Figure 2a), the flow rate is almost unchanged after formation of stable cavity. However, for higher pressure gradient (Figure 2b), sand production continues with a decreasing rate implying that the cavity is propelled gradually towards steady conditions; simultaneously, the flow rate is gradually increased to about 1.5 times the initial flow rate. Therefore, it may be concluded that high flow rate with limited sand production can be obtained by applying appropriate pressure gradient. Extension of this deduction to production in oil reservoirs leads to suggestion of allowing limited amount of sand production for increasing the oil productivity which has been recently considered by petroleum industry [27].

Figure 3a and b show the variation of cumulative weight of produced sand with time for
different values of flow rates while confining pressure was kept constant at 0.4 and 2.5 MPa, respectively. As can be seen, the numerical model predicts the increase of sand production where higher rates of fluid flow occur.

The normal production status in oil reservoirs is that, a well may produce a uniform amount of sand independent of production rate until some critical production rate is exceeded. Determination of critical flow rate is very important, because increasing the production rate above the critical rate results in strong increase of sand production rate. Critical flow can be determined from the results of numerical simulations by perusing the variation of the produced sand versus flow rate at different simulation times as depicted in Figure 4. From this figure, for flow rates higher than about 100 mm$^3$/s, the rapid increase in weight of the produced sand with time indicates that the flow rate exceeds the critical flow rate while confining pressure is equal to 0.4 MPa.
5.2 Effect of confining pressure

Previous studies show that the effect of confining pressure on arching behavior is a function of grain size distribution, particles size and dimension of the outlet opening [28, 29]. Generally speaking higher confining stresses causes increased shear strength which results in higher frictional resistance between sand particles and improving the arch stability.

The effect of confining pressure on the value of critical flow rate was studied by further analyses for two other confining stresses (2.5 and 4.4 MPa). Comparison between the results for different confining stresses (Figure 4, 5a and 5b) implies that for higher confining stresses, the rate of sand flow has been reduced. Also, the results obtained by numerical model confirm increasing the critical flow rate when higher confining pressures are applied. In Figure 6, the results of numerical simulations were compared with Al-Awad et al.’s experimental observations. Both of the curves show that increasing the confining pressure results in increasing in the critical flow rate. The higher slope of numerical curve in this figure implies that the numerical model slightly overestimates the effect of confining pressure. The reason for this different may be the 2D nature of the numerical modeling which confines the sand particles more than what occurs in the physical experiments.

Figure 4: Variation of the weight of produced sand with flow rate at different simulation times

Figure 5: Variation of the weight of produced sand with flow rate at different simulation times
5.2 Effect of confining pressure

Previous studies show that the effect of confining pressure on arching behavior is a function of grain size distribution, particles size and dimension of the outlet opening [28, 29]. Generally speaking higher confining stresses causes increased shear strength which results in higher frictional resistance between sand particles and improving the arch stability. The effect of confining pressure on the value of critical flow rate was studied by further analyses for two other confining stresses (2.5 and 4.4 MPa). Comparison between the results for different confining stresses (Figure 4, 5a and 5b) implies that for higher confining stresses, the rate of sand flow has been reduced. Also, the results obtained by numerical model confirm increasing the critical flow rate when higher confining pressure s are applied. In Figure 6, the results of numerical simulations were compared with Al -Awad et al.'s experimental observations. Both of the curves show that increasing the confining pressure results in increasing in the critical flow rate. The higher slope of numerical curve in this figure implies that the numerical model slightly overestimates the effect of confining pressure. The reason for this different may be the 2D nature of the numerical modeling which confines the sand particles more than what occurs in the physical experiments.

6 CONCLUSIONS

A coupled LB-DE model has been developed which is capable of capturing the fundamental mechanisms involved in sand production phenomenon. By using the developed code, it becomes possible to evaluate the effects of different parameters on the sand production rate/volume such as flow rate and confining stresses. Based on the conducted numerical simulations explained above, the following conclusions can be drawn:

1) The numerical model predicts the increase of sand production where higher rates of fluid flow occur.
2) The obtained results show that increasing the confining pressure results in increasing the critical flow rate which confirms the experimental observations.

REFERENCES


DEM SIMULATION OF THE MECHANICAL PROPERTIES OF SiC CERAMIC UNDER PRE-STRESSING

S.Q. JIANG*, Y.Q. TAN*, H. ZHANG*, D.M. YANG*† AND G.F. ZHANG*

* School of Mechanical Engineering
Xiangtan University, Xiangtan 411105, China
Email: jsqcx@126.com, tanyq@xtu.edu.cn

† School of Civil Engineering
University of Leeds, Leeds, LS2 9JT, UK
Email: cndy@leeds.ac.uk

Key words: DEM, Mechanical properties, SiC, Pre-stress.

Abstract. In this paper, the method of discrete element model (DEM) simulation was used to investigate the mechanical properties of SiC ceramic materials under the action of pre-stress. Using the bonded particle model (BPM), several different numerical tests (such as UCT, TPB, SENB tests) of SiC ceramic were established. Different pre-stress values were applied on the lateral surface of the ceramic specimen during the numerical simulation process, all tests were carried out at least 5 times with different random number, and the average mechanical properties results were calculated. It was showed that the existence of pre-stress has a significant effect on the mechanical properties of materials. It can enhance the strength of materials, while the force action on material in machining process force or action force the crack’s initiation and propagation was limited.

1 INTRODUCTION

Special ceramic materials such as silicon carbon, silicon nitride, alumina and zirconia are considered to be used in sealing elements, bearings, cutting tools, engine components, wear-resistant coatings and other applications for their excellent properties. Usually, the applications of ceramic materials require the parts or components with high dimensional tolerances and good surface finish. However, the hardness and brittleness of materials make the machining processing very difficult and grinding becomes one of the main machining methods. The grinding quality of ceramic components is very difficult to control because the interaction between tool and ceramic surface in grinding process can cause material damages, e.g. surface/sub-surface cracks and residual stress [1, 2]. Those damages produced by machining can be detrimental to the strength and performance of components.

Until recently, many studies of damage have been conducted with the aim to reduce machining damage. Several novel grinding technology with the applications of additional physical or chemical actions have been proposed to obtain better machining efficiency and quality, such as electrolytic in-process dressing (ELID) [3], ion beam figuring (IBF) [4], magneto-rheological finishing (MRF) [5], etc. Inspired by these applications, we argue that application of external forces or stresses, which are used to change the stresses field within
the specimen before and during the machining process, may change the final material damage mechanism. Huang et al [6] studied the effects of lateral stress in indentation experiments of rock. They found that the lateral restraint stresses can change the damage zone of the indentation, and the transverse cracks can replace the median cracks to some extent. Head and Cline [7] studied several polycrystalline ceramics of high-restraint stress in quasi-static triaxial compression experiments and found the transition phenomenon of ceramics from brittle fracture to plastic behavior. Yoshino et al. [8] studied monocrystalline silicon under hydrostatic pressure in the scratching and single-point diamond cutting and found that there was a significant improvement in the damage and surface roughness. In our earlier study, we also found that the existence of pre-stress can restrain the crack propagation and the obvious plastic deformation can be found at the bottom of scratched groove [9, 10]. However, little attention has been devoted to how the external forces or stresses affecting on the materials mechanical properties, and from the viewpoint of mechanical properties of materials, the reasons why the existence of pre-stress can reduce the machining damages are still needed to be investigated.

The purpose of this paper is to investigate how the pre-stress affecting the materials mechanical properties by discrete element model (DEM) simulations. Several different numerical tests were carried out to get the mechanical properties of SiC ceramic under the action of different pre-stress values. The results in this paper may be used to explain why the existence of pre-stress can reduce the machining damages of materials and get better surface quality of components.

2 DISCRETE ELEMENT METHOD (DEM)

DEM was firstly introduced by Cundall [11] for analysis of rock-mechanics problems. It assumes that the small particles are circular in 2D or spherical in 3D and can overlap or detach. Essentially, DEM is not based on the continuum mechanics, which is the most difference between finite element method (FEM) and discrete element method. DEM can simulate the granular material with larger deformation as well as simulating the fracture behavior of solid brittle materials, such as geo-materials [12], concrete [13, 14], ceramic [15] etc. The calculations performed in the DEM alternate between the application of Newton’s second law to the particles and a force-displacement law at the contacts. The motion equation of Newton’s second law in the DEM can be described as following:

\[ m_i \frac{dv_i}{dt} = \sum_{j=1}^{k_i} \left( F_{c,ij} + F_{d,ij} \right) + m_i g + F_i \]  
(1)

Where \( m_i \) is the mass of particle \( i \), \( v_i \) is its translational velocity and \( k_i \) is the number of particles in contact with \( i \) at time \( t \). \( F_c \) is the contact force of particle \( i \), \( F_d \) is the damping force of particle \( i \), \( m_i g \) is the gravitational force, \( F_i \) is the external force action on particle \( i \).

According to force-displacement law, the resulting contact force acting on the contact between two particles can be described as following:

\[ \vec{F} = F^n \vec{n} + F^s \vec{s} \]  
(2)

Where \( \vec{F} \) is the resulting force, \( F^n \) is the normal force and \( F^s \) is the shear force. The normal force and shear force can be calculated by

\[ F^n = K^n U^n \]  
(3)
Where \( K^n \) and \( K^s \) are the normal and shear components of the contact stiffness, \( U^s \) is the overlap between two contact particles, \( \Delta U^s \) is the shear component of the displacement.

### 3 DEM SIMULATION

#### 3.1 DEM modeling of SiC ceramic

In this paper we used the PFC2D [16] (particle flow codes in two dimensions) as the simulation platform. And the bonded-particle model (BPM) also was adopted, which can be envisioned as a kind of cemented with a finite size joining the two particles, as shown in Figure.1. A parallel bond can be regarded as a set of elastic springs with constant stiffness (normal and shear) and strength (tensile and shear), uniformly distributed over a rectangular cross-section lying on the contact plane and centered at the contact point. It can transmit both force and moment. If the maximum tensile stress exceeds the tensile strength or the maximum shear stress exceeds the shear strength, then the parallel bond breaks (represents an individual micro-crack).

Based on PFC2D, we use the specimen-genesis procedure from Augmented FishTank [16] to generate the sample of needed BPM model that is similar to the micro-structure of SiC. In order to represent the complex-shaped grains of SiC, we make a number of particles bonded into a cluster. The clustering algorithm is controlled by \( S_c \), the maximum number of particles in a cluster. Each cluster is grown by identifying the current particle as a seed particle and then adding adjacent particles to the cluster until either all adjacent particles have been added or the cluster size has reached \( S_c \). It can clearly to see that the algorithm provides no control over cluster shape but does produce a collection of complex cluster shapes that are extremely similar to the grains in a polycrystalline SiC ceramic. The results are shown in Figure.2. Here we set the maximum allowable number of particles in a cluster equal to 7, and different colors represent the different clusters.

![Fig.1 Sketch map of parallel bond.](image1)

![Fig.2 Complex-shaped grains of SiC material in PFC2D.](image2)

#### 3.2 Calibration of the DEM model of SiC ceramic

In general sense, the macro-properties of ceramics are usually described by its elastic modulus, unconfined compressive strength, Poisson’s ratio, bending strength and fracture...
toughness etc., while for codes such as PFC that synthesize macro-properties material behavior from the interactions of micro-scale components, the input properties of the microscopic constituents are usually not known. In order to have a confidence that the particular model is reproducing desired physical behavior, it is necessary to calibration the micro-parameters of DEM model. To some extent, this is a trial and error process, because there is no complete theory that can predict macroscopic behavior form microscopic properties and geometry [16]. However, this can be achieved by several numerical experiments. In this paper, the distributions of particles were random in specified region, and the average radius of particles was 2 μm. The main mechanical properties which are Young’s modulus, compressive strength, Poisson’s ratio, fracture toughness and bending strength are simulated by uniaxial compressive test (UCT), three point bending test (TPB) and single edge notched bending test (SENB). The size of DEM model for UCT test was 0.3 mm × 0.8 mm, consisting of 2077 clusters and 10267 balls. The size of DEM model of TPB and SENB tests was 1.0 mm × 0.25 mm, consisting of 2077 clusters and 10267 balls. All of the numerical tests were simulated at least 5 times with different random numbers to eliminate the impact of random errors. The numerical results of mechanical properties with comparison of experimental measurements are presented in Table 1.

Table 1. The main mechanical properties of SiC in experiment tests and in 2D DEM simulations

<table>
<thead>
<tr>
<th>Mechanical properties</th>
<th>Test results</th>
<th>DEM model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus E [Gpa]</td>
<td>420</td>
<td>425.7</td>
</tr>
<tr>
<td>Poisson’s ratio ν</td>
<td>0.14</td>
<td>0.138</td>
</tr>
<tr>
<td>Uniaxial compressive strength [Mpa]</td>
<td>2000</td>
<td>2019.8</td>
</tr>
<tr>
<td>Bending strength [Mpa]</td>
<td>500-800</td>
<td>658.1</td>
</tr>
<tr>
<td>Fracture toughness [MPa/m^1/2]</td>
<td>3.5</td>
<td>3.54</td>
</tr>
</tbody>
</table>

3.3 DEM modeling of mechanical properties of SiC ceramic with pre-stress

In order to investigate the effect of pre-stress on mechanical properties of SiC ceramic, different pre-stress values (0, 50, 100, 200, 300 and 400 MPa) were applied on the lateral surface of the ceramic specimen during the numerical simulation process, as shown in Figure 3.
Figure 3. Similarly, the numerical tests under different pre-stresses were carried out five times by changing the random number in the models. During the UCT test, the loading speed (top and bottom walls act as loading platens) is specified as 0.2 m/s, stress and strain acting throughout specimen are monitored using either wall-derived quantities or by using the stress and accumulated strains from measurement circles. The elastic modulus, unconfined compressive strength and Poisson’s ratio are calculated by the axial stress-strain curves. During the TPB test and SENB test, the loading wall is specified as 0.05 m/s, the force in Y direction is recorded automatic. The bending strength and fracture toughness are calculated according to the peak force and specimen size.

4 RESULTS AND DISCUSSION

4.1 Failure response

Figure 4 shows the axial stress-strain curves under different pre-stress values. It can be clearly to see that brittle fracture is still the main material failure mode even if under the action of pre-stress. As the increasing of pre-stress, the peak stress is also increased. However, there is a little changing in the slopes of the axial stress-strain curves under different pre-stresses. As shown in Figure 5, the Y direction force in TPB test and SENB test are increased as the increasing of pre-stress. When the applied pre-stress is 400 MPa, the peak force for both TPB and SENB test has reached 100 kN. The higher the force acting on the specimen indicates that the bending strength and fracture toughness is greater.
4.2 Mechanical properties

According to the previously mentioned failure analysis, the mechanical properties of SiC ceramic are calculated. The averages of mechanical properties are also calculated, as shown in Figure 6. It is found that the existence of pre-stress affect the mechanical properties of SiC ceramic obviously. As the increasing of pre-stress, the Poisson’s ratio of SiC ceramic was decreased, and the Young’s modulus, compressive strength, fracture toughness and bending strength were increased monotonically. That is to say, the existence of pre-stress make the SiC ceramics has enhanced strength, stiffness, and its deformability reduced. The materials under pre-stressing showed that a part of mechanical properties of ceramics make it become harder, more brittle and more strength, just like a “super-ceramic”.

The existence of pre-stress enhanced the strength and stiffness of ceramic when the pre-stress was applied on the lateral surface of materials. According to our previous studies [9, 17], the existence of pre-stress has a little effect on scratching tangential force or cutting force. It is shown that the cutting force action on the materials almost keeps the same, while the material’s strength under pre-stress was enhanced, so it can resist or limit the crack’s initiation and propagation. However, the existence of pre-stress did not increase the deformability of ceramic materials. In addition, from the results of axial stress-strain curves, it can be seen that the failure mode of ceramic under pre-stress was main brittle fracture.

![Graphs showing mechanical properties](image)

Figure 6 Effects of pre-stress on mechanical properties of SiC ceramic.
5 CONCLUSIONS
- According to UCT results with different pre-stress values, brittle fracture is still the main material failure mode.
- The existence of pre-stress has a significant effect on the mechanical properties of materials. As the increasing of pre-stress, the Poisson’s ratio of SiC ceramic was deceased, and the Young’s modulus, compressive strength, fracture toughness and bending strength were increased monotonically.
- The existence of pre-stress enhanced the strength of materials, so it can resist or limit the crack’s initiation and propagation.

ACKNOWLEDGEMENT
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REFERENCES


DETERMINATION OF THE RVE SIZE OF QUASI-BRITTLE MATERIALS USING THE DISCRETE ELEMENT METHOD

FRANCISCO MONTERO* AND FERNANDO MEDINA

*Escuela Técnica Superior de Ingenieros
Universidad de Sevilla
Camino de los Descubrimientos s/n, 41092 Seville, Spain
e-mail: fmchacon@us.es, grupo.us.es/gingest

Key words: RVE size, lattice-particle model, quasi-brittle materials, discrete element method

Abstract. Within a general multiscale scheme, it is necessary to define the representative volume element (RVE), over which a measured value becomes representative of the material. In the present work, the RVE size is determined by means of discrete element method (DEM), namely a three-dimensional lattice-particle model. These type of models have been proved to be efficient for simulating fracture processes in quasi-brittle materials. The model is used to perform the numerical simulations for different specimen sizes, aggregate distributions and material regimes. The resulting information is submitted into a statistical analysis and the chi-square test seems to be the best approach to determine the RVE size.

1 INTRODUCTION

Recent advances on computational performance have led to the development of multiscale models in order to tackle large and complex multi-field problems that were not solved formerly due to technical limitations. A wider spectrum of resolution is now available but previous studies are still necessary to carry out multiscale simulations.

Within a general multiscale scheme, the determination of the representative volume element (RVE) is of great interest. For homogenization techniques, the RVE is the cell to which homogenization is applied or the attached cell to a macro integration point in nested schemes [1].

The determination of the RVE size for random heterogeneous materials has been studied by some authors [1, 2, 3] with continuum-based models. In the present work, the discrete element method (DEM), namely a three-dimensional lattice-particle model, is used to perform the numerical simulations for cubic specimens of concrete. This type of models have been proved to be efficient for simulating fracture mechanics in cement composites.
This model has been used extensively to perform the statical procedure proposed by Gitman [2]. Two aggregate distributions are generated to study its effect on the RVE size. A simple way to apply boundary conditions by means of boundary particle is used to obtain less sparse results. Simulations are carried out until the hardening regime. RVE sizes varying from 25 mm to 100 mm are considered.

The RVE size for quasi-brittle materials has been successfully determined with the discrete element method. Results have shown a good agreement with the experimental observations and continuum-based model solutions. The main advantages of discrete models are also discussed in this work.

2 DISCRETE MODELS IN QUASI-BRITTLE MATERIALS

Several discrete models have been successfully implemented for the simulation of multiphysics problems in quasi-brittle materials. Cundall [4] discretized the continuum into circular particles with superficial interaction, with main applications in granular materials and fluid mechanics. Using a similar approach, Kawai [5] implemented the rigid-body-spring network (RBSN) to solve structural problems. Bolander [6], based on Kawai’s model, replaced the disk elements by a Voronoi tessellation to study fracture mechanics of concrete. In Zubelewicz and Bažant [7], the interacting elements are defined by the aggregates and their surrounding area.

Another type of discrete model is the lattice-based. In such a way, Bažant [8] developed a random particle model with axial interaction between the aggregates where a softening behavior is implemented. In the so-called Delft lattice model by Schlangen [9], on the other hand, the continuum is replaced by a truss whose minimum length is lower than the smallest inclusion so that different phases can be taken into account. After reaching a certain stress threshold, the failed beams are removed and microcracks are generated. Based on previous work by Bažant, Cusatis [10] presented a lattice-discrete particle model, an enhanced model achieved by implementing a more complex formulation based on the microplane models with very satisfactory results.

With the enhancement of computational power, new formulations of the problem are now possible, improving the model response. One issue concerning the discrete models is that, depending on the type, an important number of degrees of freedoms may be required. Therefore, multiscale techniques seems attractive in this case.

The authors’ lattice-particle model is based on some concepts of the aforementioned works and is successfully used to simulate fracture processes in concrete.

2.1 Material model

At the mesolevel, concrete is a random heterogeneous quasi-brittle material with three main phases: mortar, aggregates and interfacial transition zone (ITZ). In the RVE size determination, tensile tests on cubic specimens of length $D$ will be performed. This will set the domain where the aggregates must be placed. Aggregates are assumed to
be spherical-like particles and only coarse aggregates are taken into account. Particle generation is made according to a Fuller’s distribution, \( P(d) = \left(\frac{d}{d_{\text{max}}}\right)^n \), where \( P(d) \) is the cumulative percentage passing a sieve aperture diameter \( d \) with respect to the maximum aggregate size \( d_{\text{max}} \); the exponent in the equation is \( n = 0.5 \). The total volume of coarse aggregates is assumed to be 40% of the whole concrete volume [11].

Once the particle distribution is generated following the sieve curve, these are randomly placed using the take-and-place method [8]. The largest particles are placed first so that the smaller particles can be placed reasonably. A normal probability distribution is used to place the particles. For a given particle, the new position must meet the following requirements: a) not only the center but all the particle must remain inside the domain and b) particles must not overlap. The first issue is immediately satisfied by a simple coordinate transformation. For the second one, the take-and-place suggests to relocate the overlapping particles into a void.

The mesh is constructed following the actual aggregate arrangement by means of Delaunay’s triangulation (fig. 1), therefore it will only depend on the actual material mesostructure. Every connecting element represents the interaction between two particles. The area of the element is found so as to preserve the volume distribution of adjacent tetrahedra [10].

### 2.2 Elastic formulation

Every element of the mesh represents the mechanical interaction between the particles as shown in fig. 2. This is modeled by spring elements acting in normal and tangential directions, with stiffnesses: \( K_{ij}^N = k_1 E_{ij} A_{ij} / L_{ij} \) and \( K_{ij}^T = k_2 E_{ij} A_{ij} / L_{ij} \). Parameters \( k_1 \) and \( k_2 \) are used to adjust the macroscopic elastic modulus and Poisson’s ratio, respectively. In general, values of \( k_1 = 5 \) and \( k_2 = 0.3 \) lead to satisfactory results. \( A_{ij} \) and \( L_{ij} \) are directly obtained from Delaunay’s triangulation [10].

Local elastic modulus \( E \) will depend on the three phases of the heterogeneous material: mortar \( (E_m) \), aggregates \( (E_a) \) and ITZ \( (E_{ITZ}) \) [8]:

\[
\frac{L}{E} = \frac{L_{a1}}{E_a} + \frac{L_{ITZ}}{E_{ITZ}} + \frac{L_m}{E_m} + \frac{L_{a2}}{E_a} + \frac{L_{ITZ}}{E_{ITZ}}
\]  

(1)

In the numerical simulations, the material properties are:
This formulation appears to be sufficient to reproduce the mechanical behavior at the meso- and macroscale under the elastic regime.

### 2.3 Fracture behavior

Different fracture laws can be found in the literature (i.e. linear or exponential softening laws in tension, hardening rules in compression) to account for the fracture behavior. However, for the present work, a simple brittle failure law (fig. 2c) has been tested in different configurations and provided satisfactory results. Brittle failure at local scale leads to quasi-brittle failure at global scale.

For a given load step, element stresses are computed and compared to their corresponding failure surface. The element with maximum stress-to-strength ratio is supposed to fail. Since shear interaction is also present, a Mohr-Coulomb failure surface (fig. 3) is used to account for other failure modes [6]. For the simulations, the following fracture parameters are used: \( \phi = 35^\circ \), \( c = 2f_t \) and \( f_t = 4 \) MPa.

### 3 DETERMINATION OF THE RVE SIZE

Many definitions for the RVE can be found in the literature, the most important are reviewed in [2]. Although there is not a single and exact definition of the RVE for an arbitrary heterogeneous material [3], the main idea is that the RVE should be large enough to keep the microstructural (meso- in our case) information, and small enough with respect to the macroscopic structural dimensions [2]. Moreover, to determine an RVE it is necessary to have (a) statistical homogeneity and ergodicity of the material; these two properties assure the RVE to be statistically representative of the macro response, and (b) some scale \( L \) of the material domain, sufficiently large relative to the micro-scale \( d \) (inclusion size) so as to ensure the independence of boundary conditions [12].
In any case, the determination of the RVE size depends on the material under consideration and the structural sensitivity of the physical quantity that is measured [1]. The definition of the governing parameter is quite important because different governing parameters may lead to different values for the RVE size. In general, macroscopic quantities such as elastic moduli or mesoscopic quantities such as peak stress can be taken.

In the present work, the elastic and hardening regimes are accounted for, hence macroscopic and mesoscopic are used, respectively.

### 3.1 Problem description

The authors’ lattice-particle model described in section 2 is used extensively in different tension tests until the peak-load, so that elastic and hardening regime variables can be measured (fig. 4).

Four different RVE sizes are taken into account, \( D = 25, 50, 75 \) and 100 mm as represented in fig. 5; with two different aggregate distributions, \( d_{\text{max}} = \{8, 16\} \) mm referred to as \( d8 \) and \( d16 \), respectively (fig. 6).

<table>
<thead>
<tr>
<th>Aggregate distributions</th>
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<td>d (mm)</td>
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When dealing with RVE tests one main issue is the definition of the boundary conditions. Commonly used boundary conditions include (a) linear displacements, (b) uniform traction and (c) periodic boundary conditions [13]. This choice will affect the results of homogenization methods including homogenized properties [3]. In this work, the boundary conditions are imposed according to [1, 3] as shown in fig. 4a. So far, in the author’s model particles are only randomly distributed within the domain, then two ways for applying constant displacement at one end are used: (i) as a linear variation in a thick layer of the specimen [10] and (ii) through strategically placed particles at the surface, these particles are quite smaller than the others resulting in elements mostly of mortar.
Therefore, two different meshes will be obtained, as shown in fig. 7, and will be referred to as $b0$ for (i) and $b1$ for (ii).

An event-driven algorithm as in [9] is numerically implemented to solve the system until the peak-load. The stress-strain curve is obtained by homogenization of the surface reactions and the imposed displacement. From this curve, the elastic modulus $E$ and peak stress (tensile strength) $f_t$ can be obtained, the former a macroscopic quantity, the latter a mesoscopic quantity. For the statistical analysis under the elastic regime another macroscopic parameter such as Poisson’s ratio $\nu$ is considered. A simple procedure to measure $\nu$ can be found in [8, 10].

### 3.2 Material regimes

Under tensile loading, concrete is a softening material in which three different consecutive regimes are present: (i) elastic, (ii) hardening and (iii) softening until failure.
According to Gitman [2], RVE can be found both in the linear-elastic and the hardening regime. But once in the softening regime, material loses its representativity and cannot be found. This is caused by the damage localization and therefore loses statistical homogeneity. On the other hand, Nguyen [3] specifies that an RVE does exist in the post-peak regime for softening materials but it should be emphasized that in this case the RVE refers to a localization band.

In the present work, the elastic modulus $E$ is the chosen quantity for the elastic regime and the tensile strength $f_t$ for the hardening regime.

### 3.3 Statistical analysis

A statistical analysis is performed with the information provided by the previous simulations. Two series of samples are taken, corresponding to the elastic and hardening regimes. For both series, four different configurations are considered: two boundary conditions type (b0 and b1) and two aggregate distributions (d8 and d16).

For the elastic regime, four RVE sizes are produced ($D = 25, 50, 75$ and $100$ mm) and
nine tests are performed for each size. This is repeated for each configuration, resulting in a total number of 144 simulations.

On the other hand, three RVE sizes are produced ($D = 25, 50$ and $75$ mm). Since the numerical resolution under the hardening regime is computationally more expensive, only five complete tension tests are submitted to analysis. As for the elastic regime, this is repeated for each size and configuration, resulting in a total number of 60 simulations. For both regimes, a total number of 204 simulations have been carried out.

With all these data, it is now possible to perform a statistical analysis. In the literature many considerations can be found: (a) expectation can give a measure of the convergence but for some variables this is not possible; (b) standard deviation which does give a measure of how sparse the results are for a given size, but still requires a criterion and (c) chi-square which gives a measure of the deviation with respect to the mean value and can be compared to the corresponding value for a 95% accuracy test.

Let $x$ be a given variable and $\langle x \rangle$ its expectation, for a total number of realizations $n$, the chi-square value can be obtained by the following equation:

$$\chi^2 = \sum_{i=1}^{n} \frac{(x_i - \langle x_i \rangle)^2}{\langle x_i \rangle}$$

(2)

For an accuracy test of 95% and the statistical degree of freedom equal to 2, the table value is $\chi_{95\%}^2 = 0.103$. The test is positive for $\chi^2 \leq 0.103$, therefore the RVE size is found.

An RVE determination procedure is proposed in [2]. It consists of the following steps:

1. Set an initial size, $D_i = D_0$
2. Generate $n$, five at least, cubic specimens of size $D_i$
3. Perform the numerical simulations and obtain the stress-strain curve
4. Compute the corresponding $\chi^2$ value
5. Perform the accuracy test: if $\chi^2 \leq 0.103$ then RVE size is achieved: $D_i$; otherwise increase $D_i$ and go to (ii)

4 RESULTS

There are many estimations of the RVE sizes by different approaches. Generally, following a theoretical estimation, Lemaitre [14] proposed a value of 100 mm for concrete. Experimental observations [15, 16] refined the RVE size to, approximately, $D = (3 - 5) d_{max}$ and $D = (7 - 8) d_{max}$. Using the concept of characteristic length [17, 18], another value of the RVE is proposed as $D = (2.7 - 3) d_{max}$. Analytical approaches [19] suggest an RVE size to be $D = 4.5 d_{max}$.

Chi-square test results are presented below for the accounted regimes. The chosen quantities are the elastic modulus $E$ for the elastic regime and tensile strength $f_t$ for the hardening regime. Two cases are presented for each regime: b0(d8-d16), b1(d8-d16).
Figure 8: Chi-square tests for $E$ (upper), $\nu$ (medium) and $f_t$ (lower)
4.1 Elastic regime

From the results, we can clearly state that $E$ (fig. 8 - upper) seems to be a correct quantity. Results for $\nu$ (fig. 8 - medium) are also presented and shows very low values, passing the test for the first RVE size. Concerning the aggregate distribution, it can be seen that d8 converges before d16, as expected. For a same volume, d8 contains more particles allowing it to converge before. The use of boundary particles (b1) improves the results for smaller values of $D$. Boundary conditions on b0 are applied to a thick layer of particles and this is done sparsely for a low number of particles. RVE size results in 50 mm for this regime and shows a kink point at this value.

4.2 Hardening regime

In the hardening regime (fig. 8-lower), similar maximum chi-square values are obtained, although for the b0 configuration are slightly larger. In this configuration, d8 and d16 lead to similar results, but the chi-square criterion is firstly satisfied by the d8 specimen, as expected. Following this criterion, an RVE size of 45 mm results. On the other hand, for the b1 configuration this difference is larger and the RVE size for the d8 distribution is achieved from 35 mm and d16 from 45 mm.

5 CONCLUSIONS

In this paper, the determination of the RVE size in quasi-brittle materials, namely concrete, has been successfully achieved by means of a lattice-particle model developed by the authors. The determination of the RVE size is of great interest within a multiscale framework.

Following Gitman’s procedure [2], satisfactory results have been obtained for the RVE size. Results show an RVE size of $D \approx 4d_{\text{max}}$, in accordance to experimental and analytical results presented in section 4. In general, an RVE size of 50 mm seems to be a good approximation.

Two different aggregate distributions have been considered to study the dependency on the RVE size. Larger RVE sizes are obtained for larger aggregates sizes, this is more evident for the b1 series. In any case, more aggregate distributions should be considered in order to state more defined conclusions. Also, two boundary configurations have been tested. The use of boundary particles (b1) has shown to be an efficient way to obtain more converging results. This is probably due to the way boundary conditions are applied. This paper should be considered a first approach and other periodic boundary conditions should be implemented. As pointed out in [3], the size of the RVE in the case of non-periodic boundary conditions is larger and the cases with and without wall-effect are relatively similar.

Discrete element models such as the lattice-particle model are very useful to gain insight in quasi-brittle materials. Lattice-particle models results attractive in the way that a large number of degrees of freedom are decreased contrary to large continuum-based models.
The extension to softening regimes and the use of other variables such as the energy dissipation are proposed for future research.

REFERENCES


Development of discrete element approach to modeling heterogeneous elastic-plastic materials and media

Evgeny V. Shilko, Alexey Yu. Smolin, Sergey V. Astafurov and Sergey G. Paskhie

Institute of Strength Physics and Materials Science SB RAS (ISPMS SB RAS)
av. Akademicheskii 2/4, 634021 Tomsk, Russia
e-mail: shilko@ispms.tsc.ru, www.ispms.ru

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Abstract. A general approach to realization of models of elasticity and plasticity of isotropic materials within the framework of discrete element method (DEM) is proposed in the paper. It is based on building many-body potentials/forces of discrete element interaction, which provide response of element ensemble correctly conforming to the response of simulated solids. Developed formalism makes possible realization of various rheological models in the framework of DEM to study deformation and fracture of solid-phase media of various nature.

1 INTRODUCTION

An important direction in deformable solid mechanics is development of numerical methods and their application to problems connected with deformation and fracture of heterogeneous materials. A perspective and intensively developed representative of numerical methods in mechanics is a group of particle methods. At the present time this term is collective one as it includes very different numerical methods that belong both to “conventional” representatives of the discrete approach in mechanics (PM, DEM, MCA) and to meshless algorithms for numerical solution of equations of continuum (for example, particle-in-cell method [1], SPH [2], SPAM [3] and so on). Moreover, nowadays some modern realizations of conventional numerical methods (such as particle-finite element method [4]) are also referred to as particle methods. The following consideration will concern “conventional” particle methods.

In the framework of “conventional” particle methods simulated material is considered as an ensemble of interacting particles (elements) having finite size and predefined initial shape that can change as a consequence of loading. Evolution of an ensemble is defined by solution of the system of Newton-Euler motion equations:

\[
m_i \frac{d^2 \dot{R}_i}{dt^2} = \sum_{j=1}^{N_i} \left( F_{in}^j + F_{xi}^j \right)
\]

\[
J_i \frac{d^2 \dot{\theta}_i}{dt^2} = \sum_{j=1}^{N_i} M_{ij}
\]
where $\vec{r}_i$ and $\vec{\theta}_i$ are radius-vector and rotation angle of the particle $i$, $m_i$ and $J_i$ are particle mass and moment of inertia, $\vec{F}_n^{ij}$ and $\vec{F}_t^{ij}$ are forces of central (normal) and tangential interaction of considered element $i$ with neighbor $j$, $\vec{M}_{ij}$ is momentum of force, $N_i$ is a number of neighbors (conventionally only nearest neighbors of element $i$ are taken into account). It is seen from (1) that “macroscopic” (integral) properties of ensemble of elements are defined by the structure and parameters of potential (potential forces) of element interaction.

The best known representative of this group of particle methods is the discrete element method (DEM) [5,6]. At the present time DEM is widely used to study behavior of granular (loose) and weakly bonded media including features of their rheology, deformation and fracture pattern, mixing effects and so on [5-7]. Nevertheless, until recently, potentialities of application of DEM to study mechanical phenomena in consolidated medium were limited, as a rule, by porous brittle materials [5,6]. These limitations are concerned with insufficient development of mathematical models of interaction of discrete elements. In particular, overwhelming majority of models within the framework of DEM is based on use of pair-wise (two-particle) potentials/forces of element interaction. Such simplification can lead to a series of artificial manifestations (effects) of response of the ensemble of elements that are not inherent to modelled medium. Most important of them are:

- strongly pronounced dependence of macroscopic mechanical properties of ensemble of discrete elements on packing type (close, square, stochastic,…);
- inability to realize arbitrary desired ratio between macroscopic elastic moduli (shear and bulk moduli, Young modulus and Poisson ratio and so on);
- problems in correct simulation of irreversible strain accumulation in ductile materials, whose plasticity is provided by mechanisms of crystal lattice scale;
- etc.

These disadvantages are of principle for simulation of consolidated low porous materials. In this connection one of fundamental problems in DEM is formulation of interaction potentials/forces, which provide response of element ensemble conforming to response of consolidated solids with various rheological properties (elastic-plastic, visco-elastic-plastic and so on). It is clear that such potentials/forces have to have many-body form.

## 2 GENERAL FORMALISM OF MANY-PARTICLE INTERACTION

Authors propose a general approach to building many-body forces of discrete element interaction to simulate deformation and fracture of consolidated heterogeneous media. The structural form of these forces is analogous to interatomic forces calculated on the basis of embedded-atom method. In the framework of embedded-atom model [8] the general expression for potential energy of atom $i$ contains a pair interaction potential $\phi$ as a function of distance $r_{ij}$ between atoms $i$ and $j$ and a “density-dependent” embedding function $F$ (here it depends on electron charge density $\rho_i$):

$$E_i(R) = \sum_{j \neq i} \phi(r_{ij}) + \sum_{i} F(\rho_i)$$
where \( \overline{\rho}_i = \sum_{j \neq i} \rho_j \) is a sum of contributions of neighbors \( j \) to local value of density at the location of atom \( i \).

By analogy with this expression the following general form of notation of the expression for the force \( \tilde{F}_i \) acting on discrete element \( i \) from surroundings is proposed:

\[
m_i \frac{d^2 \tilde{R}_i}{dt^2} = \tilde{F}_i = \sum_{j=1}^{N_i} \tilde{F}^{ij}_{\text{pair}} + \tilde{F}^{ij}_{\Omega}
\]

This force is written as a superposition of pair-wise constituents \( \tilde{F}^{ij}_{\text{pair}} \) depending on spatial position/displacement of element \( i \) with respect to nearest neighbor \( j \) and of volume-dependent constituent \( \tilde{F}^{ij}_{\Omega} \) connected with combined influence of nearest surroundings of element.

When simulating locally isotropic media with various rheologies the volume-dependent contribution \( \tilde{F}^{ij}_{\Omega} \) can be expressed in terms of pressure \( P_i \) in the volume of discrete element \( i \) as follows [9]:

\[
\tilde{F}^{ij}_{\Omega} = -A \sum_{j=1}^{N_i} \rho S_{ij} \tilde{n}_{ij}
\]

where \( S_{ij} \) is square of area of interaction (contact) of elements \( i \) and \( j \), \( \tilde{n}_{ij} \) is a unit vector directed along the line between mass centres of considered elements, \( A \) is a parameter.

In such formulation the right part of the expression (2) can be reduced to the sum of forces of interaction of pairs of elements and divided into central \( (\tilde{F}^{ij}_n) \) and tangential \( (\tilde{F}^{ij}_\tau) \) constituents:

\[
\tilde{F}_i = \sum_{j=1}^{N_i} \left( \tilde{F}^{ij}_{\text{pair}} - AP_i S_{ij} \tilde{n}_{ij} \right) = \sum_{j=1}^{N_i} \left[ \tilde{F}^{ij}_{\text{pair,n}} (h_{ij}) - AP_i S_{ij} \tilde{n}_{ij} \right] + \tilde{F}^{ij}_{\text{pair,\tau}} (I_{\text{shear}}^{ij}) - \sum_{j=1}^{N_i} \left( \tilde{F}^{ij}_n + \tilde{F}^{ij}_\tau \right)
\]

where \( \tilde{F}^{ij}_{\text{pair,n}} \) and \( F^{ij}_{\text{pair,\tau}} \) are central and tangential components of pair-wise interaction force that depend on the values of element-element overlap \( h_{ij} \) and relative shear displacement \( I_{\text{shear}}^{ij} \) \((I_{\text{shear}}^{ij} \) is calculated taking into account rotation of both elements) [5,6]. Note that although the right part of the expression (4) formally confirms to notation of element interaction in conventional models (1) [5-7], their fundamental distinction consists in many-body form of central interaction of discrete elements in the proposed model.

It is seen from (4) that an important problem of building many-particle interaction is definition of local value of pressure \( P_i \) in the volume of discrete element. Authors propose to use an approach to calculation of pressure \( P_i \) (or, what is the same – of mean stress) in the volume of the element \( i \) that is based on the computation of components of average stress tensor in the volume of the element [6].

The case of plane motion of three-dimensional objects (quasi-two-dimensional approximation) is considered in the paper. In this approximation the expression for average stresses in terms of central \( (\tilde{F}^{ij}_n) \) and tangential \( (\tilde{F}^{ij}_\tau) \) interaction forces can be written as

follows [6]:

$$\sigma_{\alpha\beta}^{ij} = \frac{1}{V_i} \sum_{j=1}^{N_i} q_{ij} \left[ F_n^{ij} \cos \theta_{ij,\alpha} \cos \theta_{ij,\beta} \pm F_t^{ij} \cos \theta_{ij,\alpha} \sin \theta_{ij,\beta} \right]$$  \(5\)

where $\alpha, \beta = x, y$ ($XY$ is a plane of motion); $V_i$ is a current value of the volume of element $i$; $q_{ij}$ is a distance from mass centre of element $i$ to the central point of area of interaction (contact area) with neighbour $j$; $\theta_{ij,\alpha}$ is an angle between the line connecting mass centres of interacting elements $i$ and $j$ and axis $\alpha$ of laboratory system of coordinates (Figure 1). Components $\sigma_{xz}^{ij}$ and $\sigma_{yz}^{ij}$ are identically zero in the framework of considered quasi-two-dimensional approximation and definition of $\sigma_{zz}^{ij}$ depends on constitutive equations of considered medium. Note that values of $\sigma_{xy}^{ij}$ and $\sigma_{yx}^{ij}$ coincide only in static equilibrium state of ensemble of discrete elements, while they can slightly differ at the stage of establishing static equilibrium. Therefore their mean value ($\left(\sigma_{xy}^{ij} + \sigma_{yx}^{ij}\right)/2$) is used in the proposed model (hereinafter it is called as $\sigma_{xy}^{ij}$).

![Figure 1: An example of definition of angle $\theta_{ij,\alpha}$ between line connecting mass centers of discrete elements in the pair $i$-$j$ and $\alpha$-axis of laboratory system of coordinates ($\alpha=X$ is considered here). The center of coordinate system is translated to the mass center of the element $i$.](image)

Calculated in this way the stress tensor components can be used to determine the pressure in the volume of discrete element:

$$p_i = -\sigma_{\text{mean}}^{ij} = -\frac{\sigma_{xx}^{ij} + \sigma_{yy}^{ij} + \sigma_{zz}^{ij}}{3}$$  \(6\)

Note that calculated values of average stress tensor components can be used to determine other tensor invariants as well, for example stress intensity:

$$\sigma_{\text{int}}^{ij} = \frac{1}{\sqrt{2}} \sqrt{\left(\sigma_{xx}^{ij} - \sigma_{yy}^{ij}\right)^2 + \left(\sigma_{yy}^{ij} - \sigma_{zz}^{ij}\right)^2 + \left(\sigma_{zz}^{ij} - \sigma_{xx}^{ij}\right)^2 + 6\left(\sigma_{xy}^{ij}\right)^2}$$  \(7\)

It follows form (1), (4), (5) that the central problem in the framework of proposed approach to building many-body interaction of discrete element is to determine expressions for $F_n^{ij}$ and $F_t^{ij}$, which provide necessary rheological characteristics of mechanical response of ensemble of elements. Analysis of relationships (1), (4), (5) leads to the conclusion that
expressions for interaction forces could be directly reformulated from constitutive equations of considered medium (equations of state). Below is a derivation of such expressions for locally isotropic elastic-plastic materials.

3 DESCRIPTION OF ELASTIC-PLASTIC MEDIUM WITH DEM FORMALISM

For convenience hereinafter parameters of interaction of discrete elements will be considered in reduced units.

In particular, values of central and tangential relative displacements of elements of the pair \(i-j\) are distributed among them and normalized to element sizes:

\[
\Delta \varepsilon_{ij} = \frac{\Delta \varepsilon_{ij}}{\left(\frac{d_i + d_j}{2}\right)} = \frac{\Delta \varepsilon_{ij}}{d_i/2} + \frac{\Delta \varepsilon_{ij}}{d_j/2} = \Delta \varepsilon_{i(j)} + \Delta \varepsilon_{j(i)}
\]

\[
\Delta \gamma_{ij} = \frac{\Delta \gamma_{ij}}{r_{ij}} = \frac{V_{\text{shear}}^{ij} \Delta t}{r_{ij}} = \Delta \gamma_{i(j)} + \Delta \gamma_{j(i)}
\]

where symbol \(\Delta\) hereinafter indicates increment of corresponding parameter during one time step \(\Delta t\), \(r_{ij}\) is the distance between mass centers of discrete elements \(i\) and \(j\) (Figure 2), \(q_{ij}\) and \(q_{ji}\) are the distances from mass centers of elements \(i\) and \(j\) to the center of area of interaction \((q_{ij}+q_{ji}=r_{ij})\), \(d\) is size of element, \(V_{\text{shear}}^{ij}\) is a velocity of relative shear displacement of elements (it is calculated taking into account rotation of both elements [6]). Space variables \(\varepsilon_{ij}\) and \(\gamma_{ij}\) hereinafter will be called as central and shear strains of discrete element \(i\) in the pair \(i-j\).

![Figure 2: Parameters of spatial relation of the pair of discrete elements \(i\) and \(j\): distance between mass centers \((r_{ij})\) and distances from mass centers of element to the center of area of interaction \((q_{ij}\) and \(q_{ji}\)).](image)

So, in the general case strains of elements \(i\) and \(j\) in the pair \(i-j\) differ from each other. As shown below, the rule of strain distribution in the pair is inseparable linked with the expression for element interaction forces.

Forces of central \((F_n^{ij})\) and tangential \((F_t^{ij})\) interaction of discrete elements \(i\) and \(j\) will be considered in specific units:

\[
F_n^{ij} = \sigma_{ij} S_{ij}
\]

\[
F_t^{ij} = \tau_{ij} S_{ij}
\]

Specific values \((\sigma_{ij}\) and \(\tau_{ij}\)) of interaction forces will be called as central and tangential pair stresses. In accordance with (4), the general form of expressions for the central and tangential interaction forces in specific units can be written as follows:

\[
\sigma_{ij} = \sigma_{ij}^{\text{pair}} \left(\varepsilon_{ij}\right) + A \sigma_{ij}^{\text{mean}}
\]

\[
\tau_{ij} = \tau_{ij}^{pair}(\gamma_{ij})
\]

The proposed below model of elastic-plastic interaction of discrete elements will be formulated in terms of reduced values of interaction parameters.

3.1 Description of linearly-elastic medium

Stress-strain state of isotropic linearly elastic medium is described on the basis of generalized Hooke’s law. The following notation of this law will be used in the paper:

\[
\sigma_{\alpha\alpha} = 2G\varepsilon_{\alpha\alpha} + (1 - 2G/K)\sigma_{\text{mean}}
\]

\[
\tau_{\alpha\beta} = G\gamma_{\alpha\beta}
\]

where \(\alpha, \beta = x, y, z\); \(\sigma_{\alpha\alpha}\) and \(\varepsilon_{\alpha\alpha}\) are diagonal components of stress and strain tensors; \(\tau_{\alpha\beta}\) and \(\gamma_{\alpha\beta}\) are off-diagonal components; \(\sigma_{\text{mean}} = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3\) is mean stress; \(K\) is bulk modulus; \(G\) is shear modulus.

It can be seen that the form and the matter of expressions (11) for diagonal and off-diagonal stress tensor components are analogous to expressions (10) describing normal and tangential interaction of discrete elements. This leads to the simple idea to write down expressions for force response of automaton \(i\) to the impact of the neighbor \(j\) by means of direct reformulation of Hooke’s law relationships:

\[
\sigma_{ij} = 2G_i\varepsilon_{i(j)} + \left(1 - \frac{2G_i}{K_i}\right)\bar{\sigma}_{i\text{mean}}^i
\]

\[
\tau_{ij} = 2G_i\gamma_{i(j)}
\]

where \(G_i\) and \(K_i\) are shear and bulk elastic moduli of material filling the element \(i\), \(\varepsilon_{i(j)}\) and \(\gamma_{i(j)}\) are central and shear strains of element \(i\) in the pair \(i-j\), mean stress \(\bar{\sigma}_{i\text{mean}}^i\) is calculated using (6).

Proposed relationships (12) for force of element response to the impact of the neighbor \(j\) are not arbitrary. Thus, by substituting relations (6) in (4) easy to show that proposed expressions for respond force automatically provide implementation of Hooke’s law for components of average stress (\(\bar{\sigma}_{i\beta}^i\)) and strain (\(\bar{\varepsilon}_{i\beta}^i\)) tensors in the volume of element \(i\). Note that \(\bar{\varepsilon}_{i\beta}^i\) are determined by analogy with (5) in terms of strains \(\varepsilon_{i(k)}\) and \(\gamma_{i(k)}\) of the element \(i\) in pairs \(i-k\).

Proposed relationships (12) make it possible to calculate central and tangential interaction of discrete elements, whose ensemble simulates isotropic elastic medium. Taking into account the need to implement Newton’s third law for interacting pairs of discrete element (\(\sigma_{ij} = \sigma_{ji}\) and \(\tau_{ij} = \tau_{ji}\)) and the need to distribute relative displacement of elements in the pair the expressions for specific interaction forces can be written as follows:

\[
\Delta\sigma_{ij} = \Delta\sigma_{ji} = 2G_i\Delta\varepsilon_{i(j)} + \left(1 - \frac{2G_j}{K_j}\right)\Delta\bar{\sigma}_{i\text{mean}}^i = 2G_j\Delta\varepsilon_{i(j)} + \left(1 - \frac{2G_i}{K_i}\right)\Delta\bar{\sigma}_{j\text{mean}}^j
\]

\[
\Delta\varepsilon_{i(j)} \frac{d_i}{2} + \Delta\varepsilon_{j(i)} \frac{d_j}{2} = \Delta r_{ij}
\]
and

\[ \Delta \tau_{ij} = \Delta \tau_{ji} = 2G_i \Delta \gamma_{ij} = 2G_j \Delta \gamma_{ji} \]  

\[ \Delta \gamma_{i(j)} \frac{d_j}{2} + \Delta \gamma_{j(i)} \frac{d_j}{2} = v_{shear} \Delta t \]  

Here, relations for calculating the central and tangential interaction forces are written in increments (in hypoelastic form).

It should be noted that in two-dimensional formulation of the problem approximations of plane stress or plane strain state are widely used. A similar approach is used in described model:

\[ \Delta \overline{\sigma}^j_{zz} = \frac{1 - \frac{2G_i}{K_i}}{2 + \frac{2G_i}{K_i}} \left( \Delta \overline{\sigma}^j_{xx} + \Delta \overline{\sigma}^j_{xy} \right) \quad \text{plane strain} \]

\[ \Delta \overline{\sigma}^j_{zz} = 0 \quad \text{plane stress} \]

Testing results (including comparison with results obtained using the commercial software ANSYS/LS-DYNA) showed that ensemble of discrete elements that interact according to (4)-(6), (8), (9), (13)-(15), demonstrates a “macroscopically” isotropic response, even with the regular packing of elements of the same size. Note that achieving isotropic response of regularly packed elements is a fundamental problem in conventional models of DEM that use approximation of two-particle interaction.

3.2 Description of elastic-plastic medium

An important advantage of proposed approach to building many-body interaction of discrete elements is a capability to realize various models of elasticity and plasticity within the framework of DEM. In particular, a model of plastic flow (incremental plasticity) with the criterion of Mises was implemented to simulate deformation of isotropic elastic-plastic media.

For this purpose, radial return algorithm of Wilkins [10] was adopted to discrete element approach. Typically, this algorithm is formulated in terms of the stress deviator (Figure 3):

\[ \dot{\sigma} = \dot{\sigma}_0 M \]  

where

\[ \dot{\sigma}_0 = \begin{vmatrix} \sigma_x - \sigma_{cp} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \sigma_y - \sigma_{cp} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \sigma_z - \sigma_{cp} \end{vmatrix} \]

Being written in terms of stress, for components of average stress tensor in the volume of discrete element \( i \) it has the following form:

\[ \left[ \begin{array}{c} \sigma_{i,xx}^i \\ \sigma_{i,yy}^i \\ \sigma_{i,zz}^i \end{array} \right] = \left[ \begin{array}{c} \sigma_{i,xx}^{\text{mean}} - \overline{\sigma}_{i,xx} \end{array} \right] M_i + \overline{\sigma}_{i,xx}^{\text{mean}} \]

\[ \left[ \begin{array}{c} \sigma_{i,\alpha\beta}^i \\ \overline{\sigma}_{i,\alpha\beta} \end{array} \right] = \overline{\sigma}_{i,\alpha\beta} M_i \]
where $\alpha, \beta = x, y, z$ and $\alpha \neq \beta$; $(\bar{\sigma}_{\alpha \alpha}^i)$ and $(\bar{\sigma}_{\alpha \beta}^i)$ are corrected (returned) average stress tensor components; $\bar{\sigma}_{\alpha \alpha}^i$ and $\bar{\sigma}_{\alpha \beta}^i$ are stress tensor components, which result from solution of elastic problem (13)-(15) at the current time step; $M_i = \bar{\sigma}_{\alpha \alpha}^i / \bar{\sigma}_{\alpha \alpha}^{int}$ is current value of the coefficient $M$ for discrete element $i$; $\sigma_{\alpha \alpha}^{pi}$ is current radius of von Mises yield circle for the element $i$; $\bar{\sigma}_{\alpha \alpha}^{int}$ is calculated on the basis of (7) after solving elastic problem at the current time step.

![Figure 3](image)

Figure 3: Schematic representation of functioning of radial return algorithm of Wilkins. Here $\sigma_{\alpha \alpha}^{int}$ is stress intensity after elastic problem solution at the current time step.

The main problem in realization of the algorithm of Wilkins within the framework of DEM is formulation of correcting relations for element interaction forces that provide for implementation of necessary conditions of the algorithm [10]. By analogy with the elastic problem the expressions for correction of specific central and tangential forces of response of the element $i$ were derived by direct reformulation of relations (17) for average stress:

$$
\sigma'_{ij} = (\sigma_{ij} - \bar{\sigma}_{\alpha \alpha}^{mean}) M_i + \bar{\sigma}_{\alpha \alpha}^{mean}
$$

$$
\tau'_{ij} = \tau_{ij} M_i
$$

where $\sigma'_{ij}$ and $\tau'_{ij}$ are corrected specific forces.

It is easy to show that substitution of (18) in expression (5) for average stress tensor automatically provides reduction of its components to yield circle for the element $i$. This demonstrates the correctness of the proposed model.

It is necessary to note that in the general case values of reduced specific forces of response of element $i$ ($\sigma'_{ij}$ and $\tau'_{ij}$) to the impact of neighbor $j$ differ from those of element $j$ ($\sigma'_{ji}$ and $\tau'_{ji}$). In view of the need for implementation of Newton’s third law correction of specific interaction force in the pair $i-j$ has to be done with use of “united and matched” coefficient $M_i$:

$$
\sigma'_{ij} = (\sigma_{ij} - \sigma_{\alpha \alpha}^{k}) M_k + \sigma_{\alpha \alpha}^{mean}
$$

$$
\tau'_{ij} = \tau_{ij} M_k
$$

where $k = i$ or $k = j$ depending on the rule of matching of specific forces. We propose to use the minimum one of $\{M_i, M_j\}$ as the coefficient $M_k$:

$$
M_k = \min\{M_i, M_j\}
$$

where
Such “individual” approach to correction of forces of interaction of the element $i$ with different neighbours $j$ can result in divergence from rigorous satisfaction of the necessary conditions ($\overline{\sigma}_{\text{mean}}^i = \overline{\sigma}_{\text{mean}}^j$ and $\overline{\sigma}_{\text{int}}^i = M_i \overline{\sigma}_{\text{int}}^j$ [10]) of the algorithm of Wilkins. Nevertheless, testing results demonstrate that divergence from precise fulfillment of these conditions is quite small even for pairs of dissimilar elements, the elastic constants ($G$ and $K$) and hardening curves of which differ considerably.

It should be also noted that in considered two-dimensional formulation of the problem the peculiarities of the algorithm of Wilkins for approximations of plane stress or plane strain state are taken into account [10,11].

Testing results have shown that proposed model of elastic-plastic interaction of discrete elements provides good agreement of spatial distribution of stresses and strain in the ensemble of discrete elements modeling elastic-plastic medium with corresponding analytical solutions as well as with results of numerical simulation by means of commercial software ANSYS/LS-DYNA.

4 DISCRETE ELEMENT MODELS OF FRACTURE AND COUPLING

A fundamental advantage of DEM as a numerical technique is its inherent capability of direct simulation of material fracture (including multiple fracture and mixing of fragments) and coupling (cohesion) of fragments. This capability is taken into account by means of change of the state of the pair of discrete elements (“linked” pair ↔ “unlinked” pair, Figure 4a). Within the framework of conventional models of two-particle interaction of elements pair-wise force or deformation criteria of fracture are used. They are expressed in terms of critical values of central and tangential forces or relative displacements [6]. Potentialities of the developed approach to building many-body interaction of discrete elements make it possible to apply various multiparametric “force” fracture criteria (Huber-Mises-Hencky, Drucker-Prager and so on) as criteria of interelement bond breaking.
Authors propose the following method of calculating these criteria for pairs of “linked” discrete elements $i$ and $j$. It is based on determination of local values of stress tensor components at the area of interaction of considered pair $i$-$j$ (hereinafter denote this tensor as $\sigma_{ij}$) in the local coordinate system $X'Y'$ of the pair (Figure 4b). Indeed, in the coordinate system $X'Y'$ in accordance with (5) values of components $\sigma_{yy}$ and $\sigma_{yx}$ for elements $i$ and $j$ are identically equal to each other and numerically equal to specific forces of central ($\sigma_{ij}$) and tangential ($\tau_{ij}$) interaction of the elements:

$$\sigma_{yy}^{j} = \sigma_{yx}^{j} = \sigma_{yy}^{i} = \sigma_{yx}^{i} = \sigma_{ij}$$

where $\alpha' = x', y'$; $n_{\alpha'}$ are direction cosines; $f_{\alpha'}^{ij}$ are projections of specific value of interaction force vector (stress vector at the area of interaction of elements $i$ and $j$). It is evident that these values of stress tensor components can be assigned to the area of element interaction ($\sigma_{ij}$ and $\tau_{ij}$) interaction of the elements can be calculated on the basis of “lever rule”:

$$\sigma_{xx}^{ij} = \frac{\sigma_{x'x'}^{ij} q_{ji} + \sigma_{x'x'}^{j} q_{ij}}{r_{ij}}$$

where $\sigma_{xx}^{ij}$ and $\sigma_{xx}^{j}$ are components of average stress tensor in the volume of elements $i$ and $j$ in the local coordinate system of the pair.

Components $\sigma_{xx}^{ij}$, thus defined, are used to calculate necessary invariants of stress tensor which then can be used to calculate current value of applied criterion of pair fracture. In particular, below the conditions of bond breaking in the pair $i$-$j$ with use of Huber-Mises-Hencky and Drucker-Prager criteria are shown:

\[ \sigma_{ij}^{int} > \sigma_c \quad \text{Huber–Mises–Hencky criterion} \]
\[ \sigma_{ij}^{int} 0.5(a + 1) + \sigma_{ij}^{mean}1.5(a - 1) > \sigma_c \quad \text{Drucker–Prager criterion} \]

where \( \sigma_c \) is corresponding threshold value for considered pair (value characterizing strength of chemical bond), \( a \) is a ratio of material compressive strength to tensile strength, \( \sigma_{ij}^{int} \) and \( \sigma_{ij}^{mean} \) are calculated by analogy with (6)-(7).

Distinctive features of interaction of “unlinked” (i.e. contacting) elements \( i \) and \( j \), among other things, are the lack of resistance to tension (pair is considered as interacting only when \( \sigma_{ij} \leq 0 \)) and limited value of the force of tangential interaction. Maximum allowed value of tangential force in “unlinked” pairs is determined by the model of friction of surfaces of interacting elements (Amonton’s law of friction, model of Dieterich [12] and so on).

In many problems (in particular, modeling of friction pairs [13]) it is important to take into account a possibility of coupling of interacting elements (onset of cohesion in the pairs of previously “unlinked” elements). For this purpose, authors proposed some simple criteria of formation of “linked” pairs as a result of contact interaction (compression + friction) of “unlinked” elements. Examples of such criteria are: i) specific value of central force under compression (\( \sigma_{ij}^{bond} \)), where \( \sigma_{ij}^{bond} \) is threshold value for bonding; ii) pair strain under compression (\( \varepsilon_{ij}^{bond} \)), iii) friction work in considered pair taking into account the value of central interaction force (\( \sigma_c \)).

5 CONCLUSIONS

- A solution to the problem of modeling the consolidated elastic-plastic media by ensemble of discrete elements is proposed in the paper. This solution is based on use of many-particle interaction forces and on determination of volume-dependent constituent of interaction via calculation of components of average stress tensor in the volume of discrete elements. Final relations for central and tangential interaction forces are derived from constitutive rheological equations for modeled medium.

- An important advantage of the proposed expressions for element interaction is a possibility of implementation of various models of elastoplasticity or viscoelastoplasticity (which are conventionally written in terms of stress/strain tensor components) in terms of element interaction force and displacement increments. In particular, the authors realized plastic flow theory with von Mises yield criterion within the framework of DEM.

- Another important advantage of the developed formalism is a possibility to directly apply conventional multiparametric fracture criteria (Huber-Mises-Hencky, Drucker-Prager, Mohr-Coulomb etc.) as criteria of interelement bond breakage. The use of these criteria is very important for correct modeling of fracture of complex heterogeneous materials of various nature.

- At the present time described models of interaction of discrete elements are approved and widely applied to study response (including fracture) of heterogeneous materials at different scales from nanoscopic to macroscopic one. Advantages of the approach to description of elastic-plastic interaction of discrete elements makes possible
correct simulation of phenomena and processes, whose study by conventional numerical methods of continuum mechanics is difficult. The problems of this type include, for example, study of physical and mechanical processes in contact patches of technical and natural frictional pairs [13,14].

5 ACKNOWLEDGMENTS

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DISCRETE ELEMENT MODELING APPROACH TO POROSIMETRY FOR DURABILITY RISK ESTIMATION OF CONCRETE

PIET STROEVEN, NGHI L.B. LE, MARTIJN STROEVEN, LAMBERTUS J. SLUYS
Delft University of Technology, Delft, the Netherlands

Keywords: Concrete, DEM, pore connectivity, pore size distribution, porosimetry

Abstract: The paper introduces a novel approach to porosimetry in virtual concrete, denoted as random node structuring (RNS). The fresh state of this particulate material is produced by the DEM system HADES. Hydration simulation is a hybrid approach making use of well-known discretization and vector methods. Particle interferences (overlap) in the dynamic packing simulation and in the hydrating system are discussed. Assessment of pore characteristics like porosity, pore size distribution and pore connectivity are described. Particularly, the last descriptor, so crucial for durability estimation, cannot be determined explicitly in experiments.

1 INTRODUCTION

Concrete is a particulate material on different levels of its microstructure. Aggregate as a major constituent of concrete is generally packed into the dense random state, taking up about three-quarter of its volume. Various types of aggregate pack slightly differently; irregular shape and rough surface texture of crushed rock hamper particles arrive at similar maximum density as smooth-shaped and smooth-surfaced particles of fluvial origin do. This has obvious impact on mechanical properties of the composite. On micro-level, the binder particles in the fresh state of the material are packed in the watery environment to a density depending on the water to cement ratio (w/c). For the low and very low w/c ranges typical for high performance concrete (HPC), and for super-HPC, respectively, the binder particles are under the compaction by vibration regime also quite densely packed.

Volume density, shape and surface texture of the binder particles will influence the rheological properties in the fresh state. In engineering terms this is expressed by workability, compactability, or consistence, as it is presently denoted in the modern European standard for concrete. Consistence is nowadays controlled by adding chemical admixtures, however. Hence, in the fresh state the spatial dispersion of the aggregate as well as of the binder particles is the result of the geometric particle characteristics, the technological parameters (including mixture design) and the compaction by vibration regime. The dispersion characteristics are maintained during maturation of the concrete.

Dispersion characteristics of the aggregate control the size distribution of the binder pockets between the aggregate grains. Research has shown the surface-to-surface spacing with the closest neighbor to fall in a 1 and 200 µm range with an average of 50 µm, about the thickness of the Interfacial Transition Zone (ITZ). So, this corresponds to the (linear) size of the binder volume hydrating between the aggregate surfaces. During maturation, more and more pores de-percolate. This process depends on the dispersion of the cement particles,
which will be between randomness and order. Where binder particles form denser patches in
the fresh state, pore de-percolation will occur in an early state of maturation, whereas the
more dilute binder patches will lead to pore de-percolation in an advanced state of maturation
or will not de-percolated at all. Research to get insight into this phenomenon would be very
complicated, extremely time-consuming and thus expensive. Instead, discrete element
modeling (DEM) has demonstrated to offer better perspectives. This is the type of approach
followed in the research presented in this paper. For another, robotics-inspired novel approach
to porosimetry in DEM-produced concrete, see [1].

2 METHODOLOGY

DEM renders possible realistically simulating binder particle dispersion in a container that
represents the binder pocket between aggregate grains. The most frequently occurring
situation consists of two neighbor aggregate grains with other aggregate grains on somewhat
more remote locations. Hence, the prismatic container employed in DEM is traditionally
provided with two rigid surfaces facing each other and four periodic surfaces. Interfacial
transition zones (ITZs) will form at the rigid surfaces. For comparison purposes, a container
with only periodic surfaces can be used for simulating maturing paste in bulk. Quantitatively
evaluating features of gradient structures is obviously more complicated because sampling is
more complex. In experimental set ups, the researcher should delineate very narrow zones on
constant distances from the aggregate surface. The latter is already very complicated because
the aggregate grain surface is never cut over the surface normal. This leads to biases in
gradient structure observations. Moreover, to acquire enough sampling area along the
aforementioned strips for reducing scatter to acceptable proportions in observations would be
a very laborious job. Such sampling problems are readily solved in a DEM approach.

The assessment of the properties of the pore system in (partly) matured virtual cement
paste offers a complex problem. Of the relevant parameters, total porosity is the most obvious
one. Further, pore size distribution is commonly determined. However, with the eye on
durability aspects, only the percolated fraction of porosity should be of interest. So, how can
de-percolated pores are separated from pores that connect external surfaces of the paste
specimen? For this problem, Navi [2] used the discretization approach in which the specimen
is subdivided into a 3D regular lattice of cubic volume-pixels (voxels). Each voxel represents
either a solid or a pore part. Then, continuity of pores between opposite sides of the specimen
is determined by a process of clustering the voxels. Another approach, popular in various
branches of science (biology, medicine), involves slicing the specimen and checking
continuity of the pores. This serial sectioning and 3D reconstruction method was used by Ye
[3] on cement paste simulated by random sequential particle addition (RSA), so with biased
particle dispersion. Chen [4] improved the approach by using the DEM system SPACE. Of
course, results obtained by the aforementioned methods depend on the voxel size and the slice
thickness. Moreover, detection of small pores will require a large number of voxels or slices.

In this paper, a modern approach is presented for assessment of pore characteristics in
virtual cement paste. The approach is based on isotropic uniformly at random (IUR)
distributed nodes in pore space, and is therefore denoted by ‘random node structuring’ (RNS).
An advantage over the aforementioned methods is that results can be obtained with acceptable
precision without the use of a large number of nodes. Also, RNS is implemented in the DEM
system HADES, so that arbitrary shaped aggregate grains can be considered (e.g., aggregate of crushed rock or of fluvial origin). In accordance with experimental findings of Bullard and Garboczi, cement particles can be of non-spherical shape. Moreover, He [5] has also demonstrated that correct ratios of surface to volume are attainable in cases of ellipsoidal particles as well as of a mixture of different polyhedron types. Generally, shape has influence on packing density of the aggregate, and thus on dispersion and spacing of the grains. This ultimately influences size of the cement pockets and degree of ITZ overlap.

So, this paper concentrates on porosimetry by RNS in virtual cement paste. The random nodes are also employed for assessment of pore size distribution (p<sub>s, sd</sub>) by star volume measurements [6]. The isotropic random pikes of the stars centered at the nodes measure distances to pore surface. They form the basis for unbiased local volume estimation. A volume-based p<sub>s, sd</sub> is directly obtained from all measurements. Of relevance is that star volume measurements can also be applied to a set of 2D random sections.

### 2.1 Simulation of fresh cement particles by HADES

![Figure 1: Spherical particles dynamically compacted from loose (left) into dense random state (right)](image)

To obtain matured virtual cement paste, firstly, fresh cement particles need to be generated. In this research packing of fresh cement particles is simulated by HADES (HAbanera’s Discrete Element Simulator). HADES is an advanced system for making realistic particle packing simulations, also incorporating arbitrarily grains shape. HADES is a dynamic force-based system, allowing for simulating particle packing under the influence of external forces. Mechanical interaction in HADES is based on a contact mechanism algorithm that evaluates the interaction forces exerted between segments of tessellated surfaces of neighboring particles. The contact forces are functions of distances and of areas of the segments. Several forces can be applied in this way on a particle such as spring force, cohesion force, damping force and friction force. HADES renders possible implementing particle packing in containers with periodic boundaries, simulating an infinite space, with rigid boundaries, simulating aggregate’s surfaces, or with mixed conditions. Gradual reduction of container size while
particles move makes it possible achieving higher packing densities as met in practice. This is illustrated in Figure 1.

2.2 Simulation of hydration process

Several computer-based approaches for simulating the hydration process of cementitious materials have been developed in the past two decades. Bishnoi [7] classified these approaches into two categories. The first, so called ‘discretization approach’ was developed by Bentz [8-9]. The container content is subdivided into a 3D regular lattice of cubic volume-pixels (voxels), which were randomly and in proper proportion attributed to phases. A group of “similar” voxels represents a phase in a multiphase material with eventually non-spherical particles. Results are resolution-dependent. So, large numbers of voxels are required to properly represent the microstructure, appealing to computational capabilities and time investments. Also, the approach does not consider the different kinetics in the hydration process.

The second, so called ‘vector approach’ does not require a sub-division of the microstructure. The method was first used by Jennings and Johnson [10]. Hymostruc3D [11] and the Integrated Particle Kinetics Model (IPKM) [2] make use of the vector approach. Calculation of particle overlap is the most laborious stage in the vector approach. Moreover, the hydration-induced growth of the cement particles also involves complicated particle interferences. The two approaches have been combined therefore in a ‘hybrid’ system.

Initially, hydration simulation is based on the IPKM. This holds for the tri-calcium silicate (C₃S) in the fresh cement. For that purpose, the C₃S is modeled as spherical cores. As a result of the reaction with water, calcium silicate hydrate (CSH) and calcium hydroxide (CH) is formed. The CSH amount formed during a short time lap is modeled as a product layer surrounding the C₃S particle’s core. Part of the CSH amount (‘in’ product) replaces the C₃S amount that has reacted and the remaining CHS amount (‘out’ product) precipitates on the particle’s surface. The CH is assumed to either diffuse and nucleate randomly in pore space or precipitate on the surface of the existing CH grains. CH is also modeled as spherical particles. The models of different products of cement particles in the IPKM are illustrated in Figure 2.

Next, some improvements on the effects exerted by particle interferences (overlap!) are implemented by means of the discretization technique. This leads to a re-calculation of the
thickness of the new product layer on the declining free surface of the particles. The latter is determined by means of the sampling point method [12]; each particle’s surface is sampled by a number of uniformly at random distributed points [13]. The free surface fraction equals the ratio of the number of sampling points not interfering with other particles over the total number of sampling points. For an efficient checking procedure for such interferences, neighborhood should be defined. This is accomplished with the ‘cell method’ [7] (or grid subdivision method) in which the simulated space is subdivided into small cubes named ‘cell’. Each cell contains a list of the particles that interfere with the cell. Therefore, to determine which particles have to be taken into account in interference situations, only the cell as the neighborhood should be investigated. Figure 3 illustrates this for the 2D case.

For calculating the thickness of the new product layer precipitating on hydrating particles in complicated particle interference situations, an efficient numerical procedure is proposed. In it, the simulated space is sub-divided into very small cubes called ‘voxels’. Each voxel represents either one of the two possible phases, i.e., solid and pore. Each voxel’s phase is updated at each time step of the hydration process. With each trial value of the layer thickness in the iterative procedure, the number of voxels that switch from ‘pore phase’ into ‘solid phase’ due to the formation of the new layer is determined. The iterative procedure will stop when the total volume of the aforementioned switching voxels corresponds to that of the diffused product.

3 RANDOM NODE STRUCTURING (RNS) METHOD

3.1 Algorithm

RNS is a general approach, so it can be used for virtual cement paste simulated by the vector approach, the discretization approach or the aforementioned hybrid system. It starts by generating IUR dispersed nodes in container space by a pseudo-random generator algorithm. Then, the nodes situated in solid phase are eliminated from further consideration. This yields IUR dispersed nodes inside pore space as a detection system of the 3D capillary pore system.
in cement paste. The next step is a structuring process for the node system in which the relationships among the nodes are built up by unobstructed straight line segments between pairs of nodes. Figure 3 presents a 2-D scheme for RNS.

![Figure 3: 2-D scheme for RNS](image3)

When two nodes can be connected by a straight line that does not intersect with any part of the solid phases, such two nodes have ‘direct connection’. This initiates a node-clustering process. A cluster involves a group of nodes each of which is directly connected to at least one of the other nodes. When two of such clusters during this process can be directly connected between two nodes from the respective clusters, they merge into a new one. Hence, once the clustering process is finished, there are a number of structured clusters of nodes. In each of these clusters, the nodes are mutually connected, which represents the connectivity among pores in the virtual cement paste. Based on the node structure, pore characteristics such as porosity, degree of percolation, pore location distribution and pore size distribution are assessed.

### 3.2 Implementation

![Figure 5: Determination whether a point is inside or outside a polyhedron](image5)
Elimination of nodes in solid phases. As mentioned above, to obtain nodes IUR distributed in pore space, an elimination process is required of the nodes interfering with solid phase. For spherical cement particles this can easily be accomplished. For voxel-based cement particles this is also easily carried out by determining the phase of the voxel in which the considered point is situated. Figure 5 illustrates the case of a cement particle simulated by a polyhedron. A probing ray emanating from the considered node in a random direction is generated. In fact, this ray is a line segment (limited by two ends) and its length must be long enough to possibly go through the polygon. If the number of intersections of the ray and the polyhedron’s surfaces (polygons) is odd then the point is inside the polyhedron, otherwise it is outside the polyhedron.

Detection of connection between two nodes. As mentioned above, the RNS method involves an IUR system of nodes that are pair wise connected by unobstructed line segments. The line segment will be considered as being unobstructed if it does not have any intersection with neighboring particles. In the case that solid phases are spherical, the intersection detection reduces to that of a line and a sphere. In the case that the discretization approach is used for simulating the microstructure, a series of points with constant spacing is distributed along the line segment. The segment line will be unobstructed if there is no point situated in any voxel representing a solid phase. When particles have polyhedral shape, the detection procedure is the same as earlier described. Since two ends of the line segments are outside particles, the number of intersections is only either zero or an even number. If the number is zero then there is no intersection. Otherwise, such an intersection exists.

Improvements in computation with localized and parallel computing processing. The RNS method centers on finding direct connections between neighboring nodes. The cell method presented in part 2.1 is utilized for this purpose. Each cell contains a list of the particles that interfere with the cell and a list of associated nodes. The cells render possible executing localized operations to improve the speed of computation. So, the clustering process is first applied locally in each cell. Thereupon, the clustering process is applied in the whole simulated space. Moreover, since local clustering processes can be implemented independently and simultaneously, ‘parallel computing processing’, the advanced feature of some programming languages, is also applied to speed up the computations.

Detection of pore connectivity. Considering a cubic sample pocket of cement paste, two types of capillary pores can be distinguished. The percolated pores form continuous entities connecting two opposite sides of the specimen. The de-percolated pores or the isolated pores might be connected together but are not connected to both sides of the pocket. The connectivity of pores is defined as the volume ratio of percolated pores to total of capillary pores. To complete detection of pore connectivity, also nodes should be uniformly at random distributed on the opposite outer surfaces of the specimen and incorporated in the clustering process. If there is a cluster of nodes containing at least one node in both end surfaces, then this cluster represents a percolated pore channel. In analyzing characteristics of the pore system, e.g., porosity, connectivity, pore size distribution, the nodes situated in the two end surfaces are not taken into account, however.
4 MEASURING PORE SIZE

In 2D sections of real or virtual cement paste alike, the most direct way of obtaining 3D local volume information on irregularly shaped pores of is by way of the mathematical morphology operator ‘opening’ [14]. This has been demonstrated in [15-17]. The underlying requirement of structural isotropy can be expected to be violated however inside the ITZ, so the method should be applied to bulk cement only. A next option is making star volume measurements, a method widely employed in life sciences [6]. This will be discussed later.

With computer-based models to simulate the microstructure of cement paste, a 3D pore structure can be produced and visualized by either one of the earlier approaches. Hence, a direct 3D assessment method for pore size would be attractive. Ye [3,18] filled up the reconstructed pores by spheres of successively increasing size, starting from a pre-determined point. This has been indicated leading to biased results [16,19]. The earlier mentioned technique of star volume measurements can be applied in 3D, however. Applying the RNS method, we can employ the random nodes as the centers of 3D ‘stars’ in the star volume method. Then, a large number of ‘pikes’ extend from the star center in isotropic at random directions to reach the nearest pore surfaces. Each of their lengths, $l_j$, is measured, whereupon local pore volume, $V_j$, is obtained from $V_j = 4\pi l_j^2/3 (l_j^2$ stands for average of values of $l_j^2$), so that local pore size (i.e., diameter) equals $2\sqrt[3]{l_j^2}$ [6]. Next, the volume-based cumulative pore size distribution function is constructed from all local pore size measurements, whereupon the volume-based pore size distribution function, $p_{vsd}$, is obtained through differentiation of the cumulative function. This is the most appropriate method for 3D assessment of $p_{vsd}$ in virtual cement.

5 EXAMPLES

Two cubic pockets of simulated cement paste are considered in this study. The characteristics of the two pockets are shown in Table 1 (P=periodic, R=rigid boundary). Fresh cement particles were generated and packed with the HADES systems. The initial size of the pocket was eight times reduced in the dynamic packing process. Next, the hybrid hydration simulation approach described in 2.2 was implemented. Next, the pore structure of the samples is investigated by RNS at ultimate degree of hydration (DOH). Due to shortage of water for chemical reaction, the hydration process of the samples stops at ultimate DOH of 0.727.

<table>
<thead>
<tr>
<th>Table 1: Characteristics of simulated cement samples</th>
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</thead>
<tbody>
<tr>
<td>Boundary conditions</td>
</tr>
<tr>
<td>C1 6P</td>
</tr>
<tr>
<td>C2 4P + 2R</td>
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</tbody>
</table>

Figure 6 presents the nodes distributed IUR in pore space of the two cement pockets. Based on these systems, porosity of the C1 and C2 pockets was found to amount 5.57 % and
5.59 %, respectively. The associated connected pore fractions of the C1 and C2 pockets were 98.53% and 90.7%. Figure 7 shows the gradient structures of distribution of pore volume as a function of distance from the rigid surface. Figure 8 presents examples of the pore size distribution assessed by the star volume method. Figure 9 is the sensitivity analysis revealing the influence of the numbers of the IUR nodes initially generated on connected fraction of porosity in the pocket C1. It can be seen that the value of connected fraction raises with the increase of the number of nodes to reach a plateau value when the number is exceeding 1 million. The number of the IUR nodes, however, does not have much influence on the porosity and the pore size distribution. For example, the porosity is about the same for $0.2 \times 10^6$ and $2 \times 10^6$ nodes, while the pore size distribution curves for these numbers nearly coincide as shown in Figure 10.

![Figure 6: System of IUR nodes distributed in pore space of the two cement paste pockets](image)

![Figure 7: Density distribution of pore volume as function of distance from the left rigid surface](image)
Figure 8: Volume-based pore size distribution

Figure 9: Sensitivity of connected fraction of porosity on number of IUR sampling nodes

Figure 10: $p_{vd}$ functions for different numbers of sampling nodes
6 CONCLUSION

A dynamic DEM approach for simulation of fresh cement paste pocketed between aggregate grains in concrete is presented. The HADES system that is employed renders possible simulating artificial grain shape. A hybrid approach is presented for simulation of the hydration process, combining the well-known vector and Integrated Particle Kinetics approaches. Special procedures are incorporated to account for particle interference problems in the fresh and hardened states. The proposed RNS method involves generation of IUR dispersed nodes in pore space, whereupon a process of node clustering is implemented by finding straight line connections between nodes. The final state presents the full network structure of pores in the maturing cement paste. Additional application of star volume measurements at node locations leads to the pore size distribution, while porosity is governed by the relative number of nodes in pore space. Pore connectivity is derived from the network structure. Hence, all pore characteristics relevant for durability estimation can be obtained. An example demonstrated the operational capabilities of the RNS method. The approach is potentially very versatile, since different grain shapes can be considered and from the simulated cement pocket bulk data can be derived or the pocket can have ITZs near neighboring rigid aggregate grain surfaces. Compared to quantitative image analysis approaches to real concrete, the RNS approach combines economic and reliability qualities, the latter because of present-day advanced computer facilities. Moreover, it offers insight into pore connectivity that experiments cannot, or at least cannot in an equally economic and reliable way.

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EFFECT OF PARTICLE SHAPE NON-CONVEXITY ON THE RHEOLOGY OF GRANULAR MEDIA: 3D CONTACT DYNAMICS SIMULATIONS

B. Saint-Cyr*,†, E. Azéma*, J.-Y. Delenne*, F. Radjai* and P. Sornay†

*LMGC, CNRS-Université Montpellier 2, Montpellier, France. 
Baptiste.saint-cyr@univ-montp2.fr

†CEA, DEN, SPUA, LCU, F-13108 St Paul lez Durance, France

Key words: Granular Materials, particle shape, non-convexity, texture, force transmission

Abstract. We analyze the effect of particle shape non-convexity on the quasi-static behavior of granular materials by means of contact dynamics simulations. The particles are regular aggregates of four overlapping spheres described by a nonconvexity parameter depending on the relative positions of the particles. Several packings are first submitted to isotropic compression without friction. We find that, as in 2D, the solid fraction of isotropic packings increases with non-convexity up to a maximum value and then declines to be nearly equal to that of a packing composed of only spheres. It is also remarkable that the coordination number increases quickly and saturates so that the packings composed of grains with a high level of nonconvexity are looser but more strongly connected. Then, the quasi-static behavior, structural and force anisotropies are analyzed by subjecting each packing to a triaxial compression. We find that the shear strength increases with non-convexity. We show that this increase results from the presence of multiple contacts between trimers leading to enhanced frictional interlocking.

1 INTRODUCTION

Spherical or circular shape have been mostly used to investigate the rheology and microstructure of granular materials. The widespread use of this idealized shape has been motivated by the fact that the rheology is mainly governed by the collective contact interactions of the particles. Nevertheless these models are not able to reflect some of the more complex aspects of real granular media behavior, such as high shear resistance observed for angular particles [3, 8, 9] or high volumetric changes in the case of elongated particles [5].
Among the difficulties, except the fact that numerically the modeling of complex shape gives rise to various technical difficulties both geometrical and computational [6], is that 1) the shape parameters need to be defined conveniently in order to be able to generate particle shapes with continuously-variable shape parameters and 2) particle shape can be broken down into different categories: angular shape, non-convex shape, elongated shape...

In this work we focus more precisely on the effect of non-convexity on the rheology of granular media. We consider aggregates of four overlapped spheres as a 3D generalization of trimers [12] (aggregates of three overlapping disks in 2D). Our numerical approach is presented in Sec.2. We analyze the stress-strain behavior in sec.3 as well as the topology of the contact network and force transmission as a function of nonconvexity, respectively in sec.4 and 5.

2 NUMERICAL PROCEDURES

The shape of a regular aggregate composed of four spheres of radius $r$ can be characterized by considering the radius $R$ of the circumscribed sphere as compared to the radius $R'$ of the inscribed sphere; Fig. 1(a). The difference $\Delta R = R - R'$ represents the concavity of the aggregate which, by definition, corresponds to the inward deviation from the surface of the circumscribed sphere. Hence, the non-convexity $\eta$ can be defined by the ratio $\eta = \Delta R / R$. This parameter can be calculated as a function of the ratio $d/2r$, where $d$ is the distance between the center of two spheres. This definition is similar to the so-called “Riley Sphericity” used to characterize thin sections in rock mechanic [7]. This parameter varies from 0, corresponding to a sphere, to $\eta \simeq 0.76$ corresponding to an aggregate where the constituting coplanar spheres intersect themselves at a single point (i.e. $d/2r = \sqrt{3}/2$).

We used contact dynamic (CD) simulations [1, 13, 10] to compact 12 000 aggregates (48 000 spheres) by isotropic compression inside a box of dimensions $L_0 \times l_0 \times H_0$ in
which the left, bottom and background walls are fixed and the top, the right and the front walls are subjected to the same compressive stress \( \sigma_0 \). The gravity and friction coefficients \( \mu \) and \( \mu_w \) between particles and with the walls, respectively, are set to zero in order to get homogeneous and isotropic dense packings. At equilibrium, all samples were in isotropic stress state. Eight samples are prepared according to this protocol for eight values of \( \eta \in [0, 0.7] \). Figure 1(b) shows an example of packing obtained by this procedure for \( \eta = 0.4 \). The grey-level are proportional to the mean pressure. In order to avoid long-range ordering in the limit of small values of \( \eta \), we introduce a size polydispersity by taking \( R \) in the range \([R_{\text{min}}, 3R_{\text{min}}]\) and a uniform distribution of particle volume fractions. These samples are then used as initial configuration for triaxial compression tests with \( \mu = 0.4 \) between particles. A downward velocity \( v_z \) is imposed on the upper wall while keeping a constant confining stress on lateral wall.

### 3 STRESS-STRAIN BEHAVIOR

The stress tensor \( \sigma \) can be evaluated from the simulation data as an average over all the contact of the dyadic product of contact force \( f^c \) and branch vector \( \ell^c : \sigma_{\alpha \beta} = n_c \langle f^c \ell^c \rangle_c \) [1], where \( n_c \) is the number density of contacts \( c \). Under triaxial conditions with vertical compression, we have \( \sigma_1 \geq \sigma_2 = \sigma_3 \), where the \( \sigma_\alpha \) are the stress principal values. We extract the mean stress \( p = (\sigma_1 + \sigma_2 + \sigma_3)/3 \) and the stress deviator \( q = (\sigma_1 - \sigma_3)/3 \).

During shear, the shear stress jumps initially to a high value before decreasing to a nearly constant value in the steady state. The steady-state shear stress \((q/p)^*\) characterizes the shear strength of the material. According to the Mohr-Coulomb model, in triaxial geometry, the internal angle of friction, representing the shear strength of the material, is defined by \( \sin \varphi^* = 3q/(2p + q) \) [7]. Figure 2(a) shows the variation of \((q/p)^*\) and \( \sin \varphi^* \) averaged in the steady state as a function of \( \eta \). We see that both \((q/p)^*\) and \( \sin \varphi^* \) increases with \( \eta \). We also observe that the prediction of an approximation from force and fabric anisotropies, to be discussed below, provides a nice fit to the simulation data.
Figure 3: Different types of contact between two aggregates: (a) simple (s), (b) simple-double (sd) and double (d), (c) triple-double-simple (tsd), double (td), simple (ts) and (d) quadruple contacts.

Figure 4: (a) Coordination $Z$ and connectivity $Z_c$ numbers as a function of $\eta$ both at initial and residual state, (b) Proportion of $k$ each contacts in the residual state as a function of $\eta$.

Figure 2(b) displays the solid fraction $\rho$ at initial (isotropic) $\rho^0$ and critical $\rho^*$ state as a function of non-convexity $\eta$. Interestingly, the solid fraction first grows in the range $\eta < 0.3$, then it declines slowly with $\eta$ up to a value close to that for spheres for initial state and below to that of spheres for critical state. A similar unmonotonic behavior of packing fraction has been previously observed for granular packings of elongated particles such as ellipses, ellipsoidal particles, spheroid-cylinders and rounded-cap rectangles [5, 11]. This is somewhat a counterintuitive finding as the shear strength (a monotonous function of $\eta$) does not follow the trend of solid fraction (non-monotonous).

4 CONTACT vs NEIGHBOR NETWORK

A major effect of concavities is to allow for multiple contacts between two aggregates. Various kinds of contacts can occur as shown in Fig3: (1) simple contact, (2) simple-double as two simple contacts between two pairs of spheres, or double contact, defined as two contacts between one sphere of one aggregate with two spheres of another aggregate, (3) triple contacts (t) defined as a combination of simple and double contacts (tsd), or one sphere of one aggregate and three spheres of other aggregate (td) or three simple contacts (ts), and (d) quadruple (q) contacts as two times (2b) contacts. Note that, cinquuple and sixtupple are possible but very rare, as well as td and ts contacts.

Thus, given multiple contacts between aggregates, we can distinguish between the
“coordination” number $Z$ as the mean number of contact neighbors per particle (i.e. double, triple... contacts are seen as one contact), and the “connectivity” number $Z_c$ defined as the mean number of contacts per particle.

Figure 4(a) plots $Z$ and $Z_c$ both in the isotropic and residual state as a function of $\eta$. We see that $Z_c^0$ jumps from 6 for spheres to $\simeq 12$ for $\eta > 0$. Indeed, this is compatible with the isostatic nature of our packings prepared with a zero friction coefficient [2]. For frictional aggregates, in the residual state, $Z_c^*$ is less important but increases from 3.5 to 5.5 with $\eta$. Interestingly, we see also that, both in the isostatic and residual state, $Z$ remains nearly constant for $\eta > 0$. In others words, the effect of increasing nonconvexity is therefore expressed by an increasing number of multiple contacts with the same average number of neighboring aggregates and thus for large $\eta$, the packings are loose but well connected. Figure 4(b) displays the proportion of each contact type in the residual state as a function of $\eta$. By definition, all contacts are simple at $\eta = 0$. We see that the fraction of simple contacts declines as $\eta$ increases and that of multiple contacts increases at the same time. We see also that, for $\eta > 0.4$ the proportion of each contact type remains constant with $\eta$. The increasing connectivity of the particles is obviously correlated with the increase of shear strength. This is well illustrated in Fig. 5(a) which shows a map of radial forces $f_{n'} = F n'$, where $F$ is the resultant of point forces acting at their contacts between two aggregates, projected along the branch vector $n'$ (i.e. unit vector joining the centers of the two contacting aggregates). We see that stronger force chains are composed of simple contacts reinforced by double contacts, double-simple, triple and quadruple contacts.
5 FORCE TRANSMISSION AND FRICTION MOBILIZATION

The anisotropic structures seen in Fig. 5(a) can be characterized more generally through the angular dependence \(\langle f_{\nu'}(\Omega) \rangle\) and \(\langle f_{\nu}(\Omega) \rangle\) of radial and orthoradial forces along the direction \(\nu', \text{ with } f_{\nu'} = F - f_{\nu} \nu', \text{ and } \Omega = (\theta, \phi)\) the azimuthal and radial angles that define the orientations of \(\nu'\) in 3D. We can show that the mean radial and orthoradial force, \(\langle f_{\nu'} \rangle\) and \(\langle f_{\nu} \rangle\) are respectively given by:

\[
\langle f_{\nu'} \rangle = \int_{\Omega} \langle f_{\nu'}(\Omega) \rangle P_\Omega(\Omega) d\Omega \quad \text{and} \quad \langle f_{\nu} \rangle = \int_{\Omega} \langle f_{\nu}(\Omega) \rangle P_\Omega(\Omega) d\Omega,
\]

where, \(d\Omega\) is the solid angle and \(P_\Omega(\Omega)\) the angular distribution of the branch vector. Note that due to quasi-static shearing, we have \(\langle f_{\nu'} \rangle = 0\). This means that \(\langle f_{\nu}(\Omega) \rangle\) and \(P_\Omega(\Omega)\) are orthonormal. Under the axisymmetric conditions of our simulations, these angular distributions are independent of \(\phi\), so that, at leading order on the spherical harmonic basis, we have [4, 9]:

\[
\begin{align*}
(a) \quad P_\theta(\theta) &= \frac{1}{4\pi} \{1 + a'_{\nu} [3 \cos^2(\theta - \theta_0) - 1]\}, \\
(b) \quad \langle f_{\nu'}(\Omega) \rangle &= \langle f_{\nu}(\Omega) \rangle \{1 + a_{f_{\nu'}} [3 \cos^2(\theta - \theta_{f_{\nu'}}) - 1]\}, \\
(c) \quad \langle f_{\nu}(\Omega) \rangle &= \langle f_{\nu}(\Omega) \rangle a_{f_{\nu'}} \sin 2(\theta - \theta_{f_{\nu}}),
\end{align*}
\]

where, \(a'_{\nu}, a_{f_{\nu'}}\) and \(a_{f_{\nu'}}\) are the branch, radial and orthoradial force anisotropy parameters, and \(\theta_0 = \theta_{f_{\nu'}} = \theta_{f_{\nu'}} = \theta_\sigma\) the privileged directions of the corresponding angular direction coinciding with the principal direction of the shear stress. These anisotropies are interesting descriptors of granular microstructure and force transmission properties, because they underlie the different microscopic origins of shear strength. Indeed, it can be shown that the general expression of the stress tensor leads to the following simple relation [4, 9]:

\[
\frac{q}{p} \simeq 0.4(a'_{\nu} + a_{f_{\nu'}} + a_{f_{\nu'}}), \quad (3)
\]

where the cross products between the anisotropy parameters have been neglected. Figure 2(a) shows that Eq. 3 holds well for all values of \(\eta\).

Figure 5(b) shows the variation of all anisotropies averaged in the steady state as a function of \(\eta\). We see that \(a'_{\nu}\) and \(a_{f_{\nu'}}\) increases from 0.2 to 0.3 and to 0.2 to 0.4, respectively, but they saturate for \(\eta > 0.3\). The saturation of \(a'_{\nu}\) is correlated with the fact that the mean number of neighbors per particle remains nearly constant with \(\eta\). The large amplitude of \(a_{f_{\nu'}}\) reflects the fact that stronger forces chains are developed due to the increase of multiple contacts with \(\eta\). Nevertheless, as shown in Sec. 4, at larger \(\eta\) the proportion of multiple contact remains constant and thus \(a_{f_{\nu'}}\) saturate also.

In contrast, we see that \(a_{f_{\nu'}}\) increases rapidly with \(\eta\) from 0.05 for \(\eta = 0\) to be nearly equal to \(a'_{\nu}\) for \(\eta = 0.7\). Remarkably that, at the contact scale the ratio \(|f_{\nu}|/(\mu f_{\nu}) \in [0, 1]\), where \(f_{\nu}\) and \(f_{\nu'}\) are the normal and tangential forces, provides a good measure of the degree of the mobilization of friction, Eq. 2(c) thus be seen as the angular mobilization
of friction in the neighbor frame \[9, 12\]. Indeed, it is easy to see that the mean mobilization of friction is simply given by \( \langle |f_{\mu}|/|f_{\nu}| \rangle = 5a_{f\mu}/2 \). In other words, the increase of \( a_{f\mu} \) underlies an increase of the friction mobilization. In fact, with \( \eta \) much more contacts are interlocked which have to effect to freeze the relative motion of the particles, and thus to increase the proportion of sliding particles.

6 DISCUSSION AND CONCLUSION

In this paper, we applied the contact dynamics method to simulate large samples of nonconvex aggregates. A single parameter was defined to characterize shape nonconvexity and it was varied in order to investigate its effect on the shear strength, solid fraction, texture and force transmission. It was shown that the shear strength increases with nonconvexity. By distinguishing the contact network from the neighbor network we have shown that the origins of this increase result from the increase of multiple contacts between aggregate. This leads to an increase of the proportion of interlocked aggregates. As the consequence the increasing mobilization of friction force and the associated anisotropy are key effects of non-convexity.

In this article, we have developed the texture and force transmission in terms of the neighbor orientation. It will be instructive to reinterpret and to compare this result as a function of the contacts orientation. Much more work is needed in order to understand the mechanical role of each contact type on the stress transmission. An idea is to isolate the contribution of each contact on the texture and forces anisotropies. This investigation is presently underway and will be presented in a forthcoming publication.

REFERENCES


[13] For our simulations, we used the LMGC90 which is a multipurpose software developed in Montpellier, capable of modeling a collection of deformable or undeformable particles of various shapes (spherical, polyhedral, or polygonal, and non-convex) by different algorithms.
ELEMENT TEST EXPERIMENTS AND SIMULATIONS: FROM DRY TOWARDS COHESIVE POWDERS

O. I. IMOLE, N. KUMAR AND S. LUDING

Multi-Scale Mechanics, TS, CTW
University of Twente
P.O. Box 217, 7500 AE Enschede, The Netherlands
e-mail: o.i.imole@ctw.utwente.nl, s.luding@utwente.nl, www.utwente.nl/ctw/msm

Key words: DEM, Element tests, Contact Models, Cohesive Powders, Uniaxial Compression, deviatoric stress.

Abstract. Findings from experiments and particle simulations for dry and cohesive granular materials are presented with the goal to reach quantitative agreement between simulations and experiments. Results for the compressibility, tested with the FT4 Powder Rheometer are presented. The first simulation results involve the strain controlled uniaxial compression of frictionless polydisperse spheres in a biaxial box using a linear visco-elastic contact model.

As main result, the evolution of pressure as a function of volume fraction is reported. Our anisotropic, uniaxial findings compare astonishingly well with results for purely isotropic compression. Concerning the second stress response, namely anisotropy, we present the evolution of the deviatoric stress as a function of the volume fraction, which cannot be measured with the FT4 experiment, but requires a bi-axial experiment.

1 INTRODUCTION

Cohesive powders pose a lot of challenge in various industrial applications for storage, transport and bulk handling. A full understanding of their flow behaviour still remains a challenging problem. It is also known that the bulk behaviour of cohesive powders depend on the contact properties of their constituents. In order to obtain information about the material behaviour, laboratory element test are performed with a control of the stress or strain path. Alternatively, the Discrete Element Method (DEM) also provides information on the local micro-structure of powder systems.

It has been shown in Ref. [2] that isotropic and deviatoric deformation modes are pure modes while the uniaxial deformation test derives from the superposition of an isotropic and a deviatoric test. On the other hand, the biaxial tests involve mixed stress- and strain-control instead of completely prescribed strains.

The first section describes the experimental procedure and results from compressibility tests to obtain the pressure-density relation. Next, we describe the simulation procedure and show the evolution of pressure under isotropic deformation.
2 EXPERIMENTAL SET-UP AND METHODOLOGY

The experimental equipment used in this work is the FT4 powder Rheometer (Freeman technology Ltd. UK) which has been described in Ref. [3]. The FT4 Rheometer measures flowability and processability aspects of powders. Standard accessories for the compressibility test include the 50mm diameter blade, the vented piston and the 50mm bore by 50mm diameter borosilicate test vessel. One advantage of the FT4 Rheometer is the automated nature of the test procedure requiring minimal operator intervention apart from during sample preparation. A pre-conditioning cycle using the test equipment’s automatic ‘conditioning’ procedure precedes the actual compressibility test. The procedure involves the gentle movement of the conditioning blade into the test sample to gently disturb the powder bed for a user pre-defined number of cycles. This action creates a uniform, lightly packed test sample that can be readily reproduced [4]. In this study, we allow three pre-conditioning cycles before the compressibility tests are carried out.

The compressibility tests are performed on two different food powder samples, which for the sake of brevity are not analyzed beyond the few specifications given in Table 1, but are just referred to as samples I and II. Size distribution is obtained by the ‘dry dispersion module’ of the Malvern Mastersizer 2000 (Malvern Instruments Ltd., UK) while the particle density is obtained by helium pycnometry. The specific surface area is also deduced from the Malvern PSD report. The distinguishing feature of these two samples is the percentage fat content with sample II being the powder with the lower fat content, and thus weaker expected cohesion. Obviously, the fat content influences the cohesivity of the powders with samples with higher fat showing more cohesion. As stated earlier, the samples are allowed to undergo three conditioning cycles after which the samples undergo a uniaxial compression from near 0 kPa to a maximum pressure of 20 kPa. For each test, the piston penetration depth, the normal stress, bulk density and compressibility (according to the Carr Index) are automatically recorded by the test program. A more detailed description of the test procedure is reported in [5].

<table>
<thead>
<tr>
<th>Material property</th>
<th>Unit</th>
<th>Sample I (strongly cohesive)</th>
<th>Sample II (moderately cohesive)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size distribution</td>
<td>(x_{10}) (\mu m)</td>
<td>12.783</td>
<td>3.119</td>
</tr>
<tr>
<td></td>
<td>(x_{50}) (\mu m)</td>
<td>24.236</td>
<td>8.678</td>
</tr>
<tr>
<td></td>
<td>(x_{90}) (\mu m)</td>
<td>47.579</td>
<td>22.540</td>
</tr>
<tr>
<td>Particle Density</td>
<td>kg/m³</td>
<td>1436</td>
<td>1509</td>
</tr>
<tr>
<td>Specific surface area</td>
<td>m²/g</td>
<td>0.284</td>
<td>1.414</td>
</tr>
</tbody>
</table>

Table 1. Material properties data for powder samples

The result from the compressibility test of samples I and II are shown in Fig 1, where pressure is plotted against bulk density (left) and against dimensionless volume fraction defines as ratio of granular volume to the total system volume (right). The more cohesive sample I behave differently from sample II with respect to both initial density and slope of the pressure-volume fraction curve of the sample. The sample with lower fat content has a smaller initial density at the commencement of the test and subsequently different bulk density values at the same pressure levels as the other sample. The effect of cohesion can also be seen from
the slope of the two plots, i.e., the sample with higher cohesion displays larger slope (resistance to uniaxial compression). It is not expected that the powder with higher fat content (most cohesive) powder is showing higher density. The fact is that the higher fat content has not only different contact properties, but also a different size distribution etc. So the material is different in (at least) two respects, and that might explain the unexpected density behavior. This behavior of cohesive powders will be studied in more detail in the future.

Detailed study of various material parameters, including friction, rolling resistance and contact-adhesion in Refs. [7,14,15,16], where volume fractions slightly larger than 0.4 were reported, indicate that the range of experimentally observed volume fractions is quite challenging to achieve with DEM simulations and requires future work.

3 SIMULATION PROCEDURE

The Discrete Element Method (DEM) [6] was used to perform simulations in a bi-axial box. One advantage of the bi-axial box is the possibility of realizing different deformation modes with a single test experiment with a direct control of stress and strain [2,9]. In addition, laboratory experiments with the biaxial box are also feasible [8,9].

![Graph](image.png)

Fig. 1a: Plot of pressure as a function of the bulk density for the experimental samples. Fig. 1b. Plot of pressure as a function of the dimensionless volume fraction (bulk density scaled with the particle density) for the experimental samples.
As a start-up and for initial simplicity, a linear visco-elastic contact model shown in equation (1) below determines the particle contact forces in the normal direction. In order to reduce dynamical effects and shorten relaxation times, an artificial viscous background dissipation $\gamma_b$, proportional to the particle velocity is added, resembling the damping due to a background medium.

$$f^n = k\delta + \gamma\dot{\delta}$$

(1)

where $k$ is the spring stiffness, $\delta$ as the overlap between particle contacts (as shown in Fig.2) and $\dot{\delta}$ is the relative velocity in the normal direction.

3.1 Simulation parameters

Simulation parameters are, system size $N = 4913$ particles, density $\rho = 2000$ [kg/m$^3$], elastic stiffness $k_n = 10^5$ [kg/s$^2$], particle damping coefficient $\gamma = 1$ [kg/s], background dissipation $\gamma_b = 0.1$ [kg/s]. The work of [7] provides a description of these artificial units and how they can be rescaled to fit values obtained from experiments due to the simplicity of the contact model used. It should also be noted that system has average particles radius $<r> = 1$ [mm], with polydispersity quantified by the width $w = r_{max}/r_{min} = 3$ of a uniform distribution defined in [1] where $r_{max}$ and $r_{min}$ are the radius of the biggest and smallest particles respectively.

3.2 Initial configuration

The initial configuration is such that particles were randomly generated in a 3D box and isotropically compressed to a volume above the jamming volume fraction $v_0 = 0.67$. The isotropic compression stage is taken as the conditioning or preparation stage before the initiation of the test. Uniaxial compression is subsequently initiated at this point after allowing sufficient relaxation of the isotropic system. The volume fraction increases with time during compression to a maximum of $v_{max} = 0.82$ and back to the original $v_0$ (Fig. 3a).

In theory, jamming occurs at the isostatic point [1,10,11,12]. The definition of an isostatic packing excludes all particles that do not belong to the force network, i.e. particles with exactly zero contacts are excluded. Nevertheless, in addition to the particles with zero contacts, there may be particles having some finite number of contacts for some short time, which do not contribute to the mechanical stability of the packing. These particles (and those
with zero contacts) are called \textit{rattlers}. The contacts of these rattlers are transient because the repulsive contact forces push them away from the mechanically stable backbone [1]. While it is possible to check numerically the contribution of every particle to the force network [13], a less rigorous way to identify rattlers is to just count their contacts. Since frictionless particles with less than four contacts are not mechanically stable in 3 dimensional systems, they are defined as rattlers. To exclude rattlers from the system, the definition of the classical coordination number i.e. average number of contacts per particle is modified to become

\[ C := C^m = \frac{M_4}{N} \]

where \( M_4 \) is the number of contacts of particles with at least four contacts and \( N \) is the total number of particles. The corrected coordination number, defined as \( C^* := \frac{M_4}{N_4} \) where \( N_4 \) is the number of particles with at least four contacts has value equal to 6 at the isostatic point in 3 dimensions. We do not suggest that this definition of coordination number is valid for all real powders - only a starting point for frictionless materials. We use these definitions of coordination numbers to find the pressure-volume fraction relation that is discussed in next section.

Above the jamming volume fraction, contacts between the particles are deformed more and more with increasing confining pressure. The potential energy is an indicator of the overlap between particles hence its values are considerably larger than the kinetic energy above jamming (Fig. 3(b)). Relatively lower potential energy values below the jammed state (fluid state) have been reported in [1]. Hence, the ratio of the potential energy values to the kinetic energy values gives a rough indication that the system is above the jamming regime in the quasi-static state. Lower energy ratios can be obtained by performing slower rate simulations as seen in Fig. 3(b).

Fig. 3a: Evolution of volume fraction as a function of time \((t)\) for isotropic compression. Fig. 3b. Comparison of ratio of kinetic energy to the potential energy in scaled time \((t_s = t/T)\) for two uniaxial compression simulations where \( T \) is the period of one compression-decompression cycle \((E_k/E_p < 0.1 \text{ percent})\). The simulation represented by the red curve is 10 times slower than the green.
3.3 Evolution of pressure under isotropic deformation

In this section, the relation between pressure and volume fraction is studied. The non-dimensional pressure \( p \) is defined as:

\[
p = \frac{2\langle r \rangle}{3k_T} tr(\sigma)
\]  

(3)

where \( tr(\sigma) \) is the trace of the averaged stress tensor. The normalized average overlap, \( \langle \Delta \rangle_c = \delta_c/(r) \) is related to the volumetric strain under the simplifying assumption of uniform deformation in the packing as:

\[
d\langle \Delta \rangle_c = D\varepsilon_v
\]  

(4)

where \( \varepsilon_v = \varepsilon_{ii} \) is the trace of the infinitesimal strain tensor and \( D \) is a proportionality constant that depends on the size distribution. The integral of \( \varepsilon_v \), denoted by \( \varepsilon_v \), is the true logarithmic volume change of the system relative to the reference volume \( V_0 \), with corresponding reference volume fraction, \( v_0 \), which is chosen without loss of generality to be equal to the critical, jamming volume fraction \( v_0 = v_c \), so that the average normalized overlap:

\[
\langle \Delta \rangle_c = D \int_{v_0}^{v} \varepsilon_v = D\varepsilon_v = D\ln \frac{v_c}{v}
\]  

(5)

The non-dimensional pressure equation becomes:

\[
p = p_0 \frac{v_c}{v_c} (-\varepsilon_V) \left[ 1 - \gamma_p(-\varepsilon_v) \right]
\]  

(6)

and the scaled pressure is given as:

\[
p^\ast = \frac{p v_c}{v} = p_0 (-\varepsilon_v) \left[ 1 - \gamma_p(-\varepsilon_v) \right]
\]  

(7)

Fig. 4(a). Total pressure (dimension Kg/mm.s²) as a function of the volume fraction for the loading and unloading cycle Fig. 4(b). The scaled pressure as a function of the (negative) volumetric strain for the unloading cycle for an isotropic [1] and our uniaxial dataset (right).
Fig. 4(a) shows the total pressure (dimensional) as a function of the volume fraction during the loading and unloading cycles for a purely isotropic data set and our uniaxial simulation. As seen, the pressure curve during the unloading cycle shifts to the right due to hysteretic effects. Fig 4(b) shows the scaled pressure as a function of the (negative) volumetric strain with $\nu_c = 0.665$ for a comparable isotropic compression data set and the uniaxial compression set being studied. Astonishingly, analytical prediction of the scaled pressure as a function of volumetric strain for an isotropic system compares well with our uniaxial simulation where the particles are frictionless.

Other deformation rates studied collapse with the same curve for small deformations. The scaled pressure is also well represented by the linear relation $p^* \approx -p_0 \varepsilon_y$ in Eq. (6) for small deformations. The best fit quality for pressure-strain curve for the unloading cycle is obtained when Eq. (7) is used to fit the pressure disregarding the data close to jamming since those are not reliable due to dynamic effects.

For both cases (isotropic and uniaxial), the coefficients $p_0 \approx 0.039$, $\gamma_p \approx 0.011$ and $\nu_c \approx 0.665$ fit our data well with errors less than one percent for all densities.

3.4 Deviatoric stress

The average isotropic stress (pressure) is defined as:

$$p = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3}.$$  \hspace{1cm} (8)

The deviatoric stress between the moving boundary (wall with normal in z-direction) and the fixed periodic boundary walls is defined by:

$$\sigma_{DEV1} = \sigma_{zz} - \frac{\sigma_{xx} + \sigma_{yy}}{2}$$ \hspace{1cm} (9)

Also, we define the second deviatoric stress, $\sigma_{DEV2}$ between the fixed periodic boundary directions in the system as:

$$\sigma_{DEV2} = \frac{\sigma_{xx} - \sigma_{yy}}{2}.$$ \hspace{1cm} (10)

The first deviatoric stress ($\sigma_{DEV1}$) quantifies the (stress) anisotropy between the compression/de-compression direction and the non-deformed direction, while the second deviatoric stress ($\sigma_{DEV2}$) quantifies the anisotropy between the two equivalent non-deformed directions—which should be small for symmetry reasons. Fig. 5 shows the evolution of the deviatoric stress during loading and unloading. In order to compare the magnitude of $\sigma_{DEV1}$ and $\sigma_{DEV2}$ we normalize them with the isotropic pressure $p$ and plot this as a function of the volume fraction.
The second deviatoric stress variation between the fixed periodic walls in the $x$ and $y$ plane lies close to zero during the loading and unloading cycles reflecting the symmetry in $x$-$y$ directions. In contrast, $\sigma_{DEV}$ shows some interesting profile. The stress increases up to $\approx 0.12 \pm 2\%$ from the commencement of the loading cycle and thereafter remains fairly constant till the end of the loading cycle. During unloading, it decreases almost linearly until it gets to the isotropic state ($\frac{\sigma_{DEV}}{p} = 0$) and goes down further to $\approx -0.2 \pm 2\%$ relative to the start-up point. Interestingly, the isotropic-stress is not recovered when the initial value of volume fraction is reached. That is the system stays anisotropic after the complete cyclic path.
4 CONCLUSION

We have presented results from a compressibility test on two cohesive powder samples. Our experiments show effects of the fat content (cohesivity) on the pressure-density curve. Simulation results from the strain controlled uniaxial compression of frictionless polydisperse spheres have also been presented. An important result in this study is the agreement obtained for the analytical prediction of the scaled pressure as a function of volumetric strain for a purely isotropic system and our uniaxial simulation. For our system, this suggests an advantage of the ‘cheaper’ uniaxial compression over isotropic deformation. Compression is done in one direction in the former while the three walls have to be moved simultaneously in the latter. The second observation is the confirmation of symmetry in the two non-mobile directions, and the observation of particular stress anisotropy between the moving and non-moving direction.

The overall goal of this research is towards cohesive powder modelling with the discrete element method. Therefore the work presented here is the ‘start-point’ to achieve agreement between experiments and simulation. Parameter studies with isotropic test configuration [7,14,15,16] have been performed already and have to be complemented by similar studies with uniaxial configuration – first to parallel the experiments, and second to activate anisotropy. More realistic contact models to incorporate friction and cohesion need to be implemented and physical experiments on cohesive powders with the bi-axial box needs to be performed. Agreement obtained for the analytical prediction of the scaled pressure as a function of the volume fraction will be investigated for more realistic contact models. In addition, the use of simulation parameters obtained from physical experiments will be examined. Simulations and theory on different deformation modes [2] also need to be fine-tuned, other loading paths that can be realised in the bi-axial box are currently being studied.

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REFERENCES


FORMULATION AND PROCEDURE TO TREAT A DISCRETE PARTICLE MODEL AS A CONTINUUM

D. DEL OLMO* AND A. SERRANO*

* Escuela Técnica Superior de Ingenieros de Caminos, Canales y Puertos (ETSICCP)
Universidad Politécnica de Madrid (UPM)
Ciudad Universitaria, 28040 Madrid, Spain

1 INTRODUCTION

This paper continues the path opened by previously published researches related to numerical models and stress-strain behaviour discrete particle models [1], [2] and [3].

In those researches was enounced how to generate numerically a granular media, assimilating the particles to spheres and adjusting the probability of appearance of a given size according to a grain size distribution.

Afterwards, the behaviour of these generated medias was set out as stiffness matrixes systems using a non-linear law of behaviour (Hertz’s Law) and allowing the particles to slide in their relative rotations according to Coulomb’s Law. Solving the system in these conditions displacements and forces were calculated for every contact in the media. This calculus is repeated for an increasingly external load. However, this huge amount of information must be treated somehow.

This paper presents a way to solve the problem of the great quantity of information obtained from the calculi, showing a methodology to transform all this discrete particle model information into an equivalent continuum.

2 COSSEART’S DISCRETE MEDIAS

2.1 Introduction

The mechanical behavior of a body B formed by three dimension discrete particles X is going to be studied. These particles are a numerable set that interact one with each other. The particles are considered to be semi-rigid. This means that the particle’s deformation only occurs locally in the contact for effect of forces and does not deform in the rest of the particle.

The particles of this study are spheres whose radius adjust to a grain size distribution being the probability of appearance of a certain dimension, directly proportional to the quantity of retained material in that dimension.

The defined body (B) has mass, m(B). This mass is a scalar quantity and is always positive. In addition, the mass can be sum for two bodies, B1 and B2:

\[ m(B_1 + B_2) = m(B_1) + m(B_2) \]  (1)

The body B has internal structure; this means that every particle of the body has attached axis in a certain orientation to identify the displacements and the rotations. A Scheme of these axis are shown in Figure 1. Due to the attached axis every particle has a momentum Iα, because the particles are spherically shaped, the momentums around the three axes are the same and equal to \((2/5)\cdot M\cdot R^2\).
The particles $X$ that formed up the body $B$ occupy a place in space at a certain time. The space is Euclidean, this allow choosing a rectangular Cartesian coordinate system once and for all. This is what is called the Common Reference System (CRS). In addition, space has vector structure. The particles $X$ can be referred to the CRS by a position vector $\mathbf{x}$ attached to the gravity center and orientated according to the position of the axis previously defined in a certain direction $D_\alpha$. Figure 1 shows a scheme of the position vector and the orientation of the axis.

Time is a scalar and both an absolute and relative time exists. The relative time is referred to a time, $t=0$, choose once and for all. The initial time, $t=0$, constitute a reference analogous as the CRS is reference of the position in space.

2.2 The movement

The place $\mathbf{x}$, occupied by the particles $X$ in a certain time $t$ and the orientation of those particles, $D_\alpha$, is called configuration in time $t$ of the body $B$. For an instant $t$, every particle has a position $\mathbf{x}$ and an orientation $D_\alpha$.

During time a particle $X$ acquires different positions $\bar{x}$ and different orientations $d_\alpha$. The evolution of these variables are called movement laws and specifies the position and orientations of a given particle:

$$\bar{x} = \bar{x}(X, t) \quad (4)$$
$$d_\alpha = d_\alpha(X, t) \quad (5)$$

The movement laws can be then expressed:

$$\bar{x} = \bar{x}(\mathbf{x}, t) \quad (6)$$
$$d_\alpha = d_\alpha(\mathbf{x}, t) \quad (7)$$

2.3 Displacements and rotations

A particle has 6 grades of freedom; three of them are related to the displacements; and the other three to the rotations. The displacements ($u$) are calculated by subtracting the position vector $\mathbf{x}$ in the time $t$ against the position $\mathbf{x}_0$ in the time $t=0$.

$$\bar{u} = \bar{x}(X, t) - \mathbf{x}_0 \quad (8)$$

The rotations correspond to the axial vector $\mathbf{\phi}$, which is the rotation that carries de axis $D_\alpha$ from their initial positions to their final position $d_\alpha$ in time $t$. The axial vector $\mathbf{\phi}$ is equivalent to a hemi-symmetric rotation tensor $\mathbf{w}$:

$$\bar{w} = -\bar{\varepsilon} \cdot \mathbf{\phi} \quad (9)$$

Where; $\varepsilon$ is Ricci’s permutation tensor of third order.

The rotation tensor $R^{\alpha}$ of Cosserat is the one that carries the axis from $D_\alpha$ to $d_\alpha$, being:

$$d_\alpha = R^{\alpha} \cdot D_\alpha \quad (10)$$

Where; $R^{\alpha} = \exp (\bar{w})$. For small movements can be said that:

$$R^{\alpha} = I - \bar{\varepsilon} \cdot \mathbf{\phi} \quad (11)$$

$I$ is the identity tensor. Then:
Operating, an analogous expression to the one of the displacement is obtained but referred to the rotations:

\[ d^\alpha - D^\alpha = -\tilde{\varepsilon} \cdot \tilde{\phi} \cdot D^\alpha \]  

(13)

### 3 INTERACTIONS

In this point is studied the mobilized forces and the geometry of a contact between two particles after a displacement \( \tilde{\mathbf{u}} \) takes place. A particle \( I \), exerts over a particle \( 0 \) some actions that generates a normal and shear force \( \mathbf{F} \) that in local axis components can be expressed as the summation of; \( \mathbf{F}^{01}_N; \mathbf{F}^{01}_T; \) and \( \mathbf{F}^{01}_F \) and in addition produces a torque \( \mathbf{M} \) that in the same local axis can be decomposed in; \( \mathbf{M}^{01}_F; \mathbf{M}^{01}_T; \) and \( \mathbf{M}^{01}_F \). The forces mobilized in a contact are shown in Figure 3.

![Figure 3.- Mobilized forces and torques in a contact.](image)

For a certain differential variation of the relative movements between the particle \( 1 \) and the particle \( 0 \), the following actions are analyzed:

\[ d \mathbf{F} = \begin{bmatrix} d \mathbf{F}^N \\ d \mathbf{F}^T \\ d \mathbf{F}^F \end{bmatrix} \quad \text{and} \quad d \mathbf{M} = \begin{bmatrix} d \mathbf{M}^T \\ d \mathbf{M}^F \end{bmatrix} \]  

(14) and (15)

These forces appear due to the differential movements:

\[ du^0 = \begin{bmatrix} du^0_N \\ du^0_T \\ du^0_F \end{bmatrix} ; \quad du^1 = \begin{bmatrix} du^1_N \\ du^1_T \\ du^1_F \end{bmatrix} ; \quad d\phi^0 = \begin{bmatrix} d\phi^0_N \\ d\phi^0_T \\ d\phi^0_F \end{bmatrix} \quad \text{and} \quad d\phi^1 = \begin{bmatrix} d\phi^1_N \\ d\phi^1_T \\ d\phi^1_F \end{bmatrix} \]  

(16)

The following relations are verified:

\[ d \mathbf{F} = K^F \cdot du^R \]  

(17)

\[ d \mathbf{M} = K^M \cdot d\phi^R \]  

(18)

Where:

\[ du^R = du^1 - du^0 \]  

(19)

\[ du^* = du + r \cdot d\phi \]  

(20)

\[ d\phi^R = d\phi^1 - d\phi^0 \]  

(21)

\[ K^F = \begin{bmatrix} K^F_N & 0 & 0 \\ 0 & K^F_T & 0 \\ 0 & 0 & K^F_F \end{bmatrix} \quad \text{and} \quad K^M = \begin{bmatrix} K^M_N & 0 & 0 \\ 0 & K^M_T & 0 \\ 0 & 0 & K^M_F \end{bmatrix} \]  

(22) and (23)

Two different types of materials can be considered:

- Non welded: where do not exist a cohesive material joining the particles.
- Welded: where a cohesive material joins the particles.

For a non welded material the value of \( K^F_N \) can be defined by Hertz’s contact Law:

\[ K^F_N = \frac{E}{1-v^2} \frac{r_1 r_2}{r_1 + r_2} (u^1_N - u^0_N) \]  

(24)

\[ d \mathbf{F}^N = K^F_N \cdot du^N \]  

(25)

Where; \( r_1 \) and \( r_2 \) are the radius of the particles in contact; \( E \) is Young’s modulus of the material of the particles; \( v \) is Poisson’s ratios of the particle’s material; and \( u^1_N - u^0_N \) is the total relative displacement of one particle against the other.
\[ K^F_T = \alpha \cdot K^F_N \]  \hspace{1cm} (26)

Where \( \alpha \) is a coefficient that usually takes the value of 1/3.

The torque tensor can be equaled to zero because only friction can be mobilized in the contact, that is why \( K^M_T \) and \( K^F_T \) are zero. But in the future and with a research that could guarantee the results could be possible to have very slight values for \( K^M_T \) and \( K^F_T \) representing that small torques could be possible to be mobilized.

While for a welded material, particles are joined together by a cohesive material as shown in Figure 5. The stiffness coefficients are obtained using numerical methods and modelling, considering the joining material as an elastic cylinder of radius \( a \) and \( h \) height. That is to say, the stiffness coefficients are function of the ratio \( h/a; E \) and \( \nu \). Knowing these coefficients, the forces and torques can be expressed as follow:

\[ d\mathbf{F}^N = K^N_T \cdot d\mathbf{u}^N \]  \hspace{1cm} (27)
\[ d\mathbf{F}^T = K^T_T \cdot d\mathbf{T} \]  \hspace{1cm} (28)
\[ d\mathbf{M}^T = K^M_T \cdot d\mathbf{T} \]  \hspace{1cm} (29)
\[ d\mathbf{M}^F = K^F_T \cdot d\mathbf{F}^F \]  \hspace{1cm} (30)

Figure 5.- Scheme of a welded material contact.

## 4 PROPOSAL OF FORMULATION

### 4.1 Introduction

In this point is presented the proposal of formulation that can be used to treat a discrete particle model as a continuum by analyzing the media as a set of particles and as a set of particles forming a continuous material. The final results of all this method will be the stress tensor; the deformation tensor; the torque tensor and the curvature tensor.

### 4.2 Strain formulation

In order to calculate the equivalent strain tensor of the discrete particle model is necessary to consider two situations in different times, as was stated in the previous point. However, the calculi done with the model is not time dependent but loading dependent instead. This is why the time in this formulation is substituted by the value of the external load. In this way and for a predetermined configuration, a particle will be defined by its position vector \( \mathbf{X} \) for a given load and by its new position vector \( \mathbf{X} \) after having increased the external load.

If the movements of every particle are studied between one loading step and another, a displacement gradient (\( F_{ij} \) is the displacement gradient tensor) and a rotation gradient (\( K_{ij} \) is the curvature tensor) can be defined as follows:

\[ \mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \]  \hspace{1cm} (31)
\[ F_{ij} = \frac{\partial x_i}{\partial x_j} = x_{i,j} \]  \hspace{1cm} (32)
\[ \mathbf{R} = \frac{\partial \mathbf{\phi}}{\partial \mathbf{X}} \]  \hspace{1cm} (33)
\[ K_{ij} = \frac{\partial \phi_i}{\partial x_j} = \phi_{i,j} \]  \hspace{1cm} (34)

However, the movement of a particle is conditioned by all the particles that surround it. In addition, the particle does not suffer a deformation itself, although the deformation that has interest for us is the one of the media. That is why to apply this formulation is necessary to establish a set of particles to
which this methodology will be applied. These set of particles are called the contour particles.

All the mechanics concepts that will be expressed from now on are referred to a certain particle of center P. This particle should be as near as possible to the center of the media in order to not being affected by the boundary conditions.

- A fictitious sphere of radius R and center P is defined.
- The particles of the granular media will be in one of the following sets related to the fictitious sphere:
  1) Set of inside particles (I); this set is formed by all the particles inside the fictitious sphere.
  2) Set of contour particles (C); this set is formed by all the particles that are intersected by the fictitious sphere, that is to say, is formed by every sphere which surface has a part inside the sphere and the other part out of it.
  3) Set of exterior particles (E); this set is formed by all the particles that has no contact with the fictitious sphere and not belong to the set of inside particles.

The joint of particles that belong to I and C sets constitute a macro element of radius R inside the discrete media. The contacts of the exterior particles with the contour particles are called effective contacts. That is to say, an effective contact is a contact that belongs simultaneously to the set E and C.

Using (32) the displacement gradient tensor can be expressed as:

$$F_{ij} \cdot dx_j = dx_i$$  \hspace{1cm} (35)

The gradient $F_{ij}$ is the displacement gradient of a particle $i$ respect the axis $j$, being the axis centered in the particle P. That is to say, this gradient represent the variation of the relative movement of the particle $i$ respect the particle P, for two different loading values. Figure 6 shows a scheme of this situation, where; P is the center particle, 1,2 and 3 are the centers of particles of the media and belonging to the set C.

Figure 6.- Scheme of the situation of the contour particles between two different loading steps and their relative displacements.

In the other hand, the curvature tensor can be written:

$$K_{ij}dX_j = d\phi_i$$  \hspace{1cm} (36)

Considering the tensor $F_{ij}$ as the unknown factor and the particle displacements as known (for being the result of the model calculus), an error function can be defined as the difference between the theoretical displacement of a particle ($d\vec{x}^k$*) and the real displacement ($d\vec{x}^k$) using the global strain tensor.

$$E_r = d\vec{x}^k - d\vec{x}^k$$  \hspace{1cm} (37)

To obtain the displacement gradient tensor the modulus of the error must be minimized. The error of a particle $k$ will be written as follow:

$$||E_r^k|| = \sum_i (F_{ij}dX_j - dx_j)^2$$  \hspace{1cm} (38)

The error of all the particles of the set C will be expressed as:

$$E = \sum_k E_r^k = \sum_k \left( \sum_{i=1}^{n} (F_{ij}dX_j - dx_j)^2 \right)$$  \hspace{1cm} (39)

In order to minimize the error is necessary to derivate respect the displacement gradient tensor:

$$\frac{dE}{dF_{ij}} = 0$$  \hspace{1cm} (40)

$$\frac{dE}{dF_{ij}} = 2 \sum_i (F_{ij}dX_j - dx_j) dX_i = 0$$  \hspace{1cm} (41)

$$F_{ij}(\sum_i dX_j dX_s) - (\sum_i dX_i dX_s) = 0$$  \hspace{1cm} (42)
The following system of equations is obtained after having operated the minimizing procedure:

\[ F_{ij}A_{js} = H_{is} \]  \hspace{1cm} (43)

Where:

- \( F_{ij} \) is the displacement gradient tensor.
- \( A_{js} \) The summation index covers every particle of the contour.
- \( H_{is} \) The summation index covers every particle of the contour.

The unknown factor is \( F_{ij} \) and it can be finally obtained:

\[ F_{ij} = H_{is}A_{js}^{-1} \]  \hspace{1cm} (44)

Similarly as has been done with the displacement gradient tensor, the process can be repeated to obtain the curvature tensor \( K_{ij} \) rewriting the expressions (37) to (42) in terms of rotations instead of displacements using (36). The curvature tensor can be written:

\[ K_{ij}A_{js} = H_{is} \]  \hspace{1cm} (45)

Where:

- \( K_{ij} \) is the curvature tensor.
- \( A_{js} \) The summation index covers every particle of the contour.
- \( H_{is} \) The summation index covers every particle of the contour.

Clearing from (45) \( K_{ij} \) is obtained:

\[ K_{ij} = H_{is}A_{js}^{-1} \]  \hspace{1cm} (46)

In the other hand, if the stretch of an element is considered as the difference between the modulus of the distances, \( (ds^2 - dS^2) \) and according to (31) and (32) it can be said that:

\[ ds^2 - dS^2 = \left[F_{KM}F_{KM} - \delta_{KM}\right]dX^\mu dX^\kappa \]  \hspace{1cm} (47)

The deformation can be expressed:

\[ 2E = F^T \cdot F - I \]  \hspace{1cm} (48)

Where; \( E \) is the Green-Saint Venant deformation tensor; \( I \) is the identity tensor and \( F \) is the displacement gradient tensor defined in (44).

The deformation tensor \( E \) can be written in terms of the Cauchy-Green tensor [5]:

\[ C = F^T \cdot F \]  \hspace{1cm} (49)

\[ 2E = C - I \]  \hspace{1cm} (50)

Where; \( F \) is the displacement gradient tensor defined in (44); and \( C \) is the Cauchy-Green tensor.

In order to obtain the deformation tensor of the media the following process is proposed:

1) Select a particle inside the media under a certain loading, avoiding choosing a particle near the boundaries. This particle will be \( P \).
2) Generate a fictitious sphere of radius R. By doing this a set of contour particles will be defined (see Figure 4). These contour particles are the ones that are intersected by the fictitious sphere.
3) For every particle “m” belonging to the contour, its displacements and rotations are known for two different states of loading. The equations expressed in this point must be applied to these particles and between those loads.
4) The displacement gradient tensor is calculated using (44) and (46) to the contour particles using the two selected states of loading.
5) The deformation tensor is calculated using (48).

From a certain distance from the particle \( P \), it is expected that the invariants of the deformation tensor will have not a great scattering in their values, assuring that exists a global tensor of behavior of the media.

Nowadays the application of the method is under development and in the near future is expected that the first numerical results will be obtained using the generated granular materials [3].

4.3 Stress formulation

In this point a proposal of formulation to obtain an equivalent stress tensor for a discrete particle model is presented.

As was stated in the previous point, a fictitious sphere is generated and a set of particles; inside, contour and exterior, are defined. Every effective contact is determined by a position vector \( \hat{R} \), referred to the global system of axis. The action of the exterior particle over the one belonging to the
contour is exerted in the point where the effective contact takes place. In that contact exists a force \( \vec{F} \) and a torque \( \vec{M} \). Figure 7 shows a scheme of the position vector and the force and torque that occur in the effective contact.

The following conditions must be verified in order to fulfill the equilibrium:

\[
\sum_{i=1}^{n} \vec{F}_i = 0 \quad \text{(51)}
\]

\[
\sum_{i=1}^{n} (\vec{R} \times \vec{F}_i + \vec{M}_i) = 0 \quad \text{(52)}
\]

The summation index \( i \) cover all the effective contacts belonging to the fictitious sphere.

In the other hand, a plane \( \pi \) of normal \( \vec{n} \) is defined. This plane cuts the fictitious sphere, dividing it in two halves:
- The outer half fulfills \( \vec{R} \cdot \vec{n} > 0 \)
- The inner half fulfills \( \vec{R} \cdot \vec{n} < 0 \)

The exterior particles exert two unitary actions, \( \vec{a} \) and \( \vec{m} \), over the plane \( \pi \). These unitary actions have the following expressions:

\[
A \cdot \vec{a} = \sum_{i=1}^{n} \vec{F}_i \quad \text{(53)}
\]

\[
A \cdot \vec{m} = \sum_{i=1}^{n} (\vec{M}_i + \vec{R} \times \vec{F}_i) \quad \text{(54)}
\]

The summation is extended to every effective contact of the fictitious sphere of center \( P \) and radius \( R \), situated in the outer half and \( A \) is the area of the circle \( (A= \pi \cdot R^2) \).

Figure 7.- Position vector and existing forces in an effective contact.

If the outer half of the fictitious sphere is considered as a continuous surface, a summation of forces and torques can be done. By doing this summation, an average stress is obtained acting over the plane \( \pi \). In this way, if the stress tensor would exist, it will produce the following linear relation:

\[
\sigma_{ij} = T_{ij} \rho_j \quad \text{(55)}
\]

Where; \( T_{ij} \) is the Cauchy stress tensor; \( i \) is the index that indicates the orientation of the stress and \( j \) indicates de orientation of the plane where the stress is acting. That is to say, \( T_{ij} \) is used as a transformation to obtain the component parallel to \( X_i \) of the stress over the plane of normal \( n_i \). \( \sigma_{ij} \) is the tension acting over the plane \( n_i \) in the direction of the axis \( x_i \); and \( n_i \) is the normal to the plane \( j \).

If the enounced tension is extended to the whole set of particles of the contour, the average stress over a plane of certain orientation would be:

\[
\sigma^k = \frac{(\sum F_i)}{\pi R^2} \quad \text{(56)}
\]

Where: \( \sigma^k \) is the average stress over a plane of normal \( n^k \); \( F \) are the forces acting on the plane \( n^k \); and \( R \) is the radius of the fictitious sphere.

The calculus of the stress tensor is done statistically as was done for the deformation tensor using the displacement gradient tensor. In order to do this the best adjustment to the stress tensor is searched, \( \sigma^k \).

To define the error function a stress \( \sigma^k \) is calculated using (56) over a certain plane of orientation \( n^k \). The searched stress tensor \( T_{ij} \) will produce a theoretical stress \( \sigma^{k*} \) over the same plane. Both values will differ producing an error. The quadratic error of both tensions is defined as follow:

\[
e_i^k = \sigma^{k*} - \sigma^k = T_{ij} n_i^k - \sigma^k \quad \text{(58)}
\]

If the modulus of this error is raise to the second power, the average quadratic error is obtained for a certain plane \( n^k \):

\[
E^k = |e_i^k|^2 = \sum_{i=1}^{n} (T_{ij} n_i^k - \sigma^k)^2 \quad \text{(59)}
\]

The total quadratic error corresponding to “h” characteristic planes will be:

\[
E = \sum_{k=1}^{n} E^k = |e_i^k|^2 = \sum_{k=1}^{n} \left( \sum_{i=1}^{n} (T_{ij} n_i^k - \sigma^k)^2 \right) \quad \text{(60)}
\]
To obtain the stress tensor, the error must be minimized:
\[
\frac{dE_\varepsilon}{d\tau_{ij}} = 0 \tag{61}
\]
\[
\frac{dE_\sigma}{d\tau_{ij}} = 2 \sum (T_{is}n_i^k - \sigma_j) n_j^k \tag{62}
\]
\[
T_{ij}(\sum_{k=1}^{13} n_i^k n_j^k) - (\sum_{k=1}^{13} \sigma_i^k n_j^k) = 0 \tag{63}
\]
This equality can be rewritten as:
\[
T_{ij}(\sum_{k=1}^{h} n_i^k n_j^k) = (\sum_{k=1}^{h} \sigma_i^k n_j^k) \tag{64}
\]
\[
T_{is} A_{sj} = H_{ij} \tag{65}
\]
Where:
- \(T_{is}\) is the equivalent stress tensor of the media.
- \(A_{sj} = (\sum_{k=1}^{h} n_i^k n_j^k)\) The \(k\) index covers the \(h\) planes, while \(s\) and \(j\) covers all the particles belonging to the contour.
- \(H_{ij} = (\sum_{k=1}^{h} \sigma_i^k n_j^k)\) The \(k\) index covers the \(h\) planes, while \(s\) and \(j\) covers all the particles belonging to the contour.

The unknown factor is \(T_{ij}\) and it can be finally obtained:
\[
T_{ij} = H_{is} A_{js}^{-1} \tag{66}
\]
It is expected that from a certain distance from the particle \(P\), the invariants of the stress tensor will not have a great scattering in their values, assuring that a global tensor of behavior of the media exists.

Nowadays the application of the method is under development and in the near future is expected that the first numerical results will be obtained using the generated granular materials [3].

Similarly to the formulation that has been written for the stress tensor, a formulation for the torque tensor can be enounced:
\[
M_{ij} = H_{is}^{M} A_{js}^{-1} \tag{67}
\]
Where:
- \(M_{ij}\) is the torque tensor.
- \(H_{is}^{M} = (\sum_{k=1}^{h} m_i^k n_j^k)\) The \(k\) index covers the \(h\) planes, while \(s\) and \(j\) covers all the particles belonging to the contour.
- \(A_{js}^{M} = (\sum_{k=1}^{h} n_i^k n_j^k)\) The \(k\) index covers the \(h\) planes, while \(s\) and \(j\) covers all the particles belonging to the contour.

4.4 Quality of the adjustment
To obtain a measure of the quality of the adjustment, once the stress tensor has been calculated using (66), it can be inserted in the expression of the total quadratic error (60). In this way, a value of the average quadratic error for a given load will be calculated:
\[
E = \sum_k \sum_i \left(\frac{T_{ij} n_i^k - \sigma_j}{T_{ij} n_i^k}\right)^2 \tag{68}
\]
But in our opinion is better to obtain an average value of the unitary error, being this error:
\[
E_u = \frac{1}{k} \sum_k \sum_i \left(1 - \frac{\sigma_j}{T_{ij} n_i^k}\right)^2 \tag{69}
\]
Where; \(k\) is the number of characteristic planes used for the calculi.

5 ENERGY FORMULATION
5.1 Initial ideas
In this point a formulation to study how the energy is given to the media by increasing the external load and how it is invested into the system by using the first principle of thermodynamics. Using the macroelement of radios \(R\) and centered in \(P\) defined in previous points (as if it were a body), for the development of this formulation the particles belonging to the exterior (\(E\) set); the contour (\(C\) set) and the interior (\(I\) set) are used. Figure 8 shows a scheme of the variables that will be used from now on. These variables as can be seen in Figure 8 are:
- The contour particle \(K\).
- The effective contact (as defined previously) $K_i$ that belongs to the particle $K$.
- $\mathcal{F}^{K_i}$ is the force that is acting in the effective contact. This force is formed up by a normal and a shear force as has been stated in previous points.
- $\mathcal{M}^{K_i}$ is the torque that is acting in the effective contact. This torque is formed up by a normal and a shear torque as was shown in Figure 1.
- $u^K$ are the displacements of the particle $K$ that produce the forces $\mathcal{F}$.
- $\phi^K$ are the rotations of the particle $K$ that generates the torques $\mathcal{M}$.

![Figure 8.- Scheme of forces and displacements in an effective contact of a macroelement.](image)

Applying the first principle of thermodynamics:

$$\mathcal{K} + \dot{\mathcal{E}} = P^c + P^d + \dot{Q}$$  \hspace{1cm} (70)

Where; $\mathcal{K}$ is the material derivative of the kinetic energy respect time; $\dot{\mathcal{E}}$ is the material derivative of the internal energy respect time; $P^c$ is the potential energy of the contour forces ($\mathcal{F}$ and $\mathcal{M}$) belonging to the effective contacts (defined in previous points); $P^d$ is the potential energy of the volumetric forces; and $\dot{Q}$ is the velocity of supply of heat to the body.

Using D’Alambert’s principle can be said that:

$$\mathcal{K} + P^c + P^d + \dot{p}^i = 0$$  \hspace{1cm} (71)

Where; $\dot{p}^i$ is the potential energy of the interior forces ($\mathcal{F}$ and $\mathcal{M}$) of the existing contacts of the interior particles with the contour particles of the macroelement.

Equaling (70) to (71), the resulting equation allows clearing the concept of internal energy:

$$\dot{\mathcal{E}} = Q - \dot{p}^i$$  \hspace{1cm} (72)

For the case of study, the energy consumption in the macroelement is admitted to be:
- $P^d = 0$ because there are not volumetric forces.
- $\mathcal{K} = 0$ because the loading process is very slow and it can be considered almost static.

With these suppositions result that:

$$\dot{\mathcal{E}} = P^c + \dot{Q}$$  \hspace{1cm} (73)

$$P^c = -\dot{p}^i$$  \hspace{1cm} (74)

5.2 The discrete media

As has been said in the previous point, two different potential energies associated to two set of particles must be studied; the potential energy of the contour forces; and the potential energy of the inside forces.

A) Potential energy of the contour forces

For a certain particle $K$ that belongs to the contour set (C set) and has an effective contact $K_i$, the potential energy for that particle is called $P^{ck}$. This potential has the expression:

$$P^{ck} = \sum_i \left[ \mathcal{F}^{K_i} \cdot \hat{u}^k + \mathcal{M}^{K_i} \cdot \hat{\phi}^k \right] = \left( \sum_i \mathcal{F}^{K_i} \right) \cdot \hat{u}^k + \left[ \sum_i \left( \mathcal{M}^{K_i} + \mathcal{F}^{K_i} \wedge \mathcal{F}^{K_i} \right) \right] \cdot \hat{\phi}^k$$  \hspace{1cm} (75)

The total potential energy for the whole set of particles of the contour with effective contacts will be:

$$P^c = \sum_k P^{ck}$$  \hspace{1cm} (76)

The summation of $k$ is extended to the particles $K$ of the contour. In the other hand, the total
potential energy can be factorized as:

\[ p^c = p^{cu} + p^{cf} \]  
\[ p^{cu} = \sum_k (\sum_i (\bar{F}^{ki}) \cdot \dot{\bar{u}}^k) \]  
\[ p^{cf} = \sum_k (\sum_i (\bar{M}^{ki} + \bar{r}^k \wedge \bar{F}^{ki})) \cdot \dot{\bar{\phi}}^k \]  

B) Potential energy of the inside forces

From the first principle of thermodynamics has been obtained (74) but it can be deduced directly saying that the effect of the potential energy of the inside forces \( P^i \) can be expressed:

\[ p^i = p^{ii} + p^{ic} \]  

Where; \( P^{ii} \) is the potential energy of all the contacts that belongs to a particle of the inside set and are not in contact with a particle of the contour set; \( P^{ic} \) is the potential energy of all the contacts that belongs to a particle of the inside set and are in contact with a particle of the contour set.

For a certain contact between two particles (1 and 2) and using the action-reaction law, it is known that in that contact:

\[ \bar{F}^1 + \bar{F}^2 = 0 \]  
\[ \bar{M}^1 + \bar{M}^2 = 0 \]  
\[ p^{ii} = \sum_k \left[ \sum_i (\bar{F}^{ki}) \cdot \dot{\bar{u}}^k + \sum_i (\bar{M}^{ki} + \bar{r}^k \wedge \bar{F}^{ki}) \dot{\bar{\phi}}^k \right] \]  

The inside particles are all in equilibrium, that is to say:

\[ \sum_i (\bar{F}^{ki}) = 0 \]  
\[ \sum_i (\bar{M}^{ki} + \bar{r}^k \wedge \bar{F}^{ki}) = 0 \]  

So it can be said that:

\[ p^{ii} = 0 \]  

Analogous at has been done for the inside particles, for the particles that belongs to the \( P^{ic} \) set can be expressed the potential energy of the inside effective contacts as:

\[ p^{ic} + p^c = 0 \]  
\[ p^{ic} = -p^c \]  
\[ p^i = p^{ic} = -p^c \] <C.Q.D.>  

5.3 The continuous media

In this point, the media will be considered as a continuous media and will be used the formulation proposed in the previous points.

In the macroelement of radious R (body B) that was defined, we were able to calculate as has been stated in previous points of this paper, the following:

- The tensors \( T \) and \( M \) in the field of stresses.
- The tensors \( F \) and \( K \) in the field of deformations.
- The displacements \( u \) and the rotations \( \phi \).

Both the potential energy of the contour forces and the potential energy of the inside forces will be studied as was done in point 5.3.

The potential energy of the contour forces, \( P^c \) is expressed:

\[ P^c = \int_{dB} \left( \dot{u} \cdot \sigma + \dot{\phi} \cdot \mathbf{m} \right) da = \int_{dB} \left[ \dot{u} \cdot (T \cdot n) + \dot{\phi} \cdot (M \cdot n) \right] da = \int_{dB} (\dot{u} \cdot T + \dot{\phi} \cdot M) \cdot n da \]  

Using the Gauss-Ostrogradsky theorem (Divergence theorem) (90) can be rewritten:

\[ p^c = \int_B \left[ T : \nabla \dot{u} + M : \nabla \dot{\phi} \right] dV + \int_B \left[ (\nabla \cdot \nabla) \dot{u} + (M \cdot \nabla) \dot{\phi} \right] dV \]  
\[ p^c = \int_B \left[ T : (\nabla \dot{u} + \epsilon \dot{\phi}) + M : \nabla \dot{\phi} \right] dV + \int_B \left[ (\nabla \cdot \nabla) \dot{u} + (M \cdot -\epsilon T ) \dot{\phi} \right] dV \]  

Considering that do not exist volumetric forces inside the body B (macroelement) the equilibrium equations of Cosserat’s media will be:

\[ T \nabla \dot{u} = 0 \] and \[ M \nabla - \epsilon T = 0 \]  

Substituting in (92) it is finally obtained that:

\[ p^c = \int_B \left[ T : (\nabla \dot{u} + \epsilon \dot{\phi}) + M : \nabla \dot{\phi} \right] dV = \frac{4\pi R^3}{3} \left[ T : (\nabla \dot{u} + \epsilon \dot{\phi}) + M : \nabla \dot{\phi} \right] \]  

In Cosserat’s medias is fundamental the relative stretch tensor, \( e \):

\[ e = F - R^c \]  

Where; \( R^c \) is \( R^c = \exp (-\epsilon \dot{\phi}) \), considering that the deformation is a finite deformation.
If the deformation is considered to be small it can be approximated by; \( R^c = I - \epsilon \phi \).
After this it can be formulated that:
In addition:

\[ e = F - I + \varepsilon \phi = \nabla u + \varepsilon \phi \quad (95) \]

Taking into account this tensor \( e \) and the tensor \( K \) that was defined in (46), \( P^e \) can be rewritten as:

\[ P^e = \frac{4nR^3}{3}(T; \dot{e} + M; \dot{K}) \quad (98) \]

Considering the expression (89) the potential of the inside forces can be written as:

\[ P^i = -\frac{4nR^3}{3}(T; \dot{e} + M; \dot{K}) \quad (99) \]

5.4 Results adjustments

As was stated previously and using (77), (89) and (99) the following expression relates the potential energy of the inside forces of the continuous media to the potential of the contour forces of the discrete media:

\[ \frac{4nR^3}{3} \left( T; \dot{e} + M; \dot{K} \right) = \sum_k \left[ \sum_i (\tilde{F}^{ki}) \cdot \tilde{u}^k + \sum_i (\tilde{M}^{ki} + \tilde{\phi}^k) \cdot \tilde{\phi}^k \right] \quad (100) \]

Both members of (100) can be calculated separately and independently by considering the media first as a continuous medium and then as a discrete particle media. By doing this calculus and comparing the results obtained from the continuous point of view and from the discrete approach an adjustment of the statistic values of the average tensors \( T, e, M \) and \( K \) can be done. Defining a parameter, \( \lambda^2 \), to represent the quality of the adjustment:

\[ \lambda^2 = \frac{\rho^c}{\rho^i} = \frac{\frac{4nR^3}{3} \sum_k \left[ \sum_i (\tilde{F}^{ki}) \cdot \tilde{u}^k + \sum_i (\tilde{M}^{ki} + \tilde{\phi}^k) \cdot \tilde{\phi}^k \right]}{[T; e + M; K]} \quad (101) \]

The tensors can be rewritten as follow:

\[ T^* = \lambda \cdot T \quad M^* = \lambda \cdot M \quad \dot{e}^* = \lambda \cdot \dot{e} \quad K^* = \lambda \cdot K \quad (102) \]

Another possibility to adjust the result would be to establish two different correction factors, \( \lambda_\phi \) and \( \lambda_\phi \), depending on if the correction is done in the field of movements or in the field of rotations, respectively.

5.5 Analysis of the work

The program that has been developed loads a discrete particle media with a certain load \( L \), that can be; an isotropic compression; an oedometric load; etc... This load cannot be applied directly. The load must be applied iteratively and in defined increments. This incremental loading process allows identifying which contacts develop plastic movements and which not.

It can be assumed that the load is a time function. If the loading steps would be of the same quantity it could be possible to establish a relation between the load and the time. Being:

\[ \dot{L} = \frac{dL}{dt} \]

\[ L = \int_0^t \dot{L} \, dt = \int_0^t dL = \sum \Delta L \quad (104) \]

Where the integral is related to the continuous loading in time and the summation is related to the incremental loading process.

To obtain the work done by the contour particles using the potential energy of the \( C \) set particles (\( P^c \)) is used the expression (77). This allows us to analyze the work done due to the displacement and the rotation of a particle of the medium.

In the plane of contact, \( K_i \) (contour particle \( K \) and effective contact \( i \) belonging to that particle) the increment of internal work \( \Delta W \) due to the increment of external load \( \Delta L \) is the addition of every partial increment of the work done by the components \( \Delta W_{u_i} \) and \( \Delta W_{\phi_i} \). These increments are produced by the forces \( F \) and by the torques \( M \) acting over the particle \( K \) and in the contact \( i \) after having moved \( (du) \) and rotate \( (d\phi) \) by effect of the external load. Translating this into mathematical language:

\[ \Delta W = \Delta W_u + \Delta W_\phi \quad (105) \]

\[ \Delta W_{uF} = F_n \cdot du \quad (106) \]

\[ \Delta W_{uT} = F_T \cdot du \quad (107) \]

\[ \Delta W_{\phiMP} = (\tau \wedge F_T + M_F) \cdot d\phi \quad (108) \]

\[ \Delta W_{\phiMT} = M_T \cdot d\phi \quad (109) \]
Knowing that:

\[ r \mathbf{N} = 0 \]  

(110)

These distinctive components of the work can be plastic or elastic. The following hypotheses have been done in the model and impact on the different values of the components of the work that had been defined:

- The component \( \Delta W_{\text{NF}} \) is always elastic, because the law of behavior that defines the normal force is Hertz’s Law (1) which is an elastic law although it is a non-linear law. In future improvements of the model this restriction will be deleted.

- The other three components of the work \( \Delta W_{\text{FT}}, \Delta W_{\phi MF} \) and \( \Delta W_{\phi MF} \) elastic or plastic depending on if the values of \( F_T, M_F \) and \( M_T \) have reached the limit conditions expressed in (3) and (10) to (15), respectively, or not.

Finally, the total work done by the system can be decomposed into an elastic work and a plastic work. Expressing this:

\[ \Delta W = \Delta W^E + \Delta W^P \]  

(111)

The total work, \( \Delta W^T \) can be written as:

\[ \Delta W^T = \Delta W_0^E + \Delta W_\phi^E + \Delta W_0^P + \Delta W_\phi^P \]  

(112)

6 CONCLUSIONS

This paper presents a proposal of formulation to calculate the stress, torque, deformation and curvature tensor for discrete particle medias, welded or non-welded, in order to study them as if they were continuous.

The appliance of this formulation is conditioned to that the output variables from the discrete particle model are: displacements and rotations of the particles in addition to forces and torques in every existing contact.

The enounced equations use classical mechanical concepts and statistical criteria for minimum squared adjustments.

With this methodology the knowledge acquired from the mechanical variables of a discrete particle model (forces, torques, displacements and rotations) can be changed into continuous mechanical concepts (stress, deformations and curvatures) creating a statistical mechanic of the discrete particle models.

This mechanic contribute to create a theory to facilitate future developments related to internal analysis of granular and particle medias, such as pyroclastic rocks, macroporous rocks and coarse granular materials.

In addition to the mechanical concepts a different approach is presented using the first thermodynamic principle. The statistical average tensor are adjusted with a different process as was enounced using the mechanical point of view.

7 REFERENCES


MODELLING AND SIMULATION OF THE EFFECT OF BLAST LOADING ON STRUCTURES USING AN ADAPTIVE BLENDING OF DISCRETE AND FINITE ELEMENT METHODS

CARLOS LABRA∗, EUGENIO OÑATE∗, FRANCISCO ZÁRATE∗, JERZY ROJEK∗†

∗ Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE)
Universitat Politècnica de Catalunya (UPC)
Campus Nord UPC, 08034 Barcelona, Spain
e-mail: clabra@cimne.upc.edu, onate@cimne.upc.edu, zarate@cimne.upc.edu, www.cimne.com/

† Institute of Fundamental Technological Research
Polish Academy of Sciences
Swietokrzyska 21, PL-00049, Warsaw, Poland
e-mail: jrojek@ippt.gov.pl

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Abstract. We present a new computational model for predicting the effect of blast loading on structures. The model is based in the adaptive coupling of the finite element method (FEM) and the discrete element method (DEM) for the accurate reproduction of multifracturing and failure of structures under blast loading. In the paper we briefly describe the basis of the coupled DEM/FEM technology and demonstrate its efficiency in its application to the study of the effect of blast loading on a masonry wall, a masonry tunnel and a double curvature dam.

1 INTRODUCTION

The paper presents a procedure for modelling and simulation of the effect of blast loading on structures via the adaptive coupling of the discrete element method and the finite element methods. The theoretical formulation of the discrete element method using spherical or cylindrical particles is briefly reviewed. The finite element equations for structural dynamics are integrated using a standard explicit time integration scheme. The formulation of an adaptive multiscale DEM/FEM model employing the DEM and FEM in different subdomains of the same body is presented. An overlap zone in the DEM and FEM domains is introduced adaptively in order to provide a smooth transition from one discretization method to the other. Coupling between the DEM and FEM overlapping
subdomains is provided by kinematic constraints imposed via a penalty function method. The efficiency of the new DEM/FEM method is demonstrated in its application to the study of the effect of blast loading on a masonry wall, a masonry tunnel and a double curvature concrete dam.

2 DISCRETE ELEMENT METHOD FORMULATION

The discrete element method (DEM) is widely recognized as a suitable tool to model geomaterials. This procedure can also be effectively used to model multifracture in “continuum” structures modelled as a collection of discrete elements. Formulation of spherical discrete elements following the main assumptions of Cundall [1, 2] has been developed by Oñate and Rojek [5] and Rojek and Oñate [8, 9] and implemented in an explicit dynamic formulation. The DEM assumes that the solid material can be represented as a collection of rigid particles (spheres or balls in 3D and discs in 2D) interacting with each other in the normal and tangential directions at the contact points. Material deformation is assumed to be concentrated at the contact points. Appropriate contact laws allow us to obtain desired macroscopic material properties. The contact law used takes into account cohesive bonds between rigid particles. Cohesive bonds can be broken, thus allowing to simulate fracture of material and its propagation.

2.1 Equations of motion

The translational and rotational motion of rigid spherical (3D) or cylindrical (2D) elements (particles) is described by means of the standard equations of rigid body dynamics. For the \( i \)-th element we have

\[
m_i \ddot{\mathbf{u}}_i = \mathbf{F}_i, \quad I_i \dot{\omega}_i = \mathbf{T}_i
\]  

where \( \mathbf{u} \) is the displacement of the element centroid in a fixed (inertial) coordinate frame \( \mathbf{X} \), \( \omega \) – the angular velocity, \( m \) – the element mass, \( I \) – the moment of inertia, \( \mathbf{F} \) – the resultant force, and \( \mathbf{T} \) – the resultant moment about the central axes. Vectors \( \mathbf{F} \) and \( \mathbf{T} \) include all external forces and moments applied to the \( i \)-th element, contact forces due to interactions with neighboring element and other obstacles, as well as forces resulting from damping in the system.

The equations of motion (1) are integrated in time using an explicit central difference scheme. For the \( i \)-th element this gives:

\[
\ddot{\mathbf{u}}_i^n = \frac{\mathbf{F}_i^n}{m_i}, \quad \dot{\mathbf{u}}_i^{n+1/2} = \dot{\mathbf{u}}_i^{n-1/2} + \ddot{\mathbf{u}}_i^n \Delta t, \quad \mathbf{u}_i^{n+1} = \mathbf{u}_i^n + \dot{\mathbf{u}}_i^{n+1/2} \Delta t.
\]  

The first two steps in the integration scheme for the rotational motion are identical to those given by Equation (2):

\[
\dot{\omega}_i^n = \frac{\mathbf{T}_i^n}{I_i}, \quad \omega_i^{n+1/2} = \omega_i^{n-1/2} + \dot{\omega}_i^n \Delta t.
\]  

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The vector of incremental rotation $\Delta \boldsymbol{\theta} = \{\Delta \theta_x \Delta \theta_y \Delta \theta_z\}^T$ is calculated as $\Delta \boldsymbol{\theta}_i = \omega_i^{n+1/2} \Delta t$.

Knowledge of the incremental rotation suffices to update the tangential contact forces. It is also possible to track the rotational position of particles, if necessary. The rotation matrices between the moving frames embedded in the particles and the fixed global frame are updated incrementally using a multiplicative scheme [5, 8, 9].

2.2 Contact search algorithm

Changing contact pairs of elements during the analysis process must be automatically detected. The simple approach to identify interaction pairs by checking every sphere against every other sphere would be very inefficient, as the computational time is proportional to $n^2$, where $n$ is the number of elements. In our formulation the search is based on quad-tree and oct-tree structures. In this case the computation time of the contact search is proportional to $n \ln n$, which allows to solve large frictional contact systems.

2.3 Evaluation of contact forces

Once contact between a pair of elements is detected, the forces occurring at the contact point are calculated. The interaction between the two interacting bodies can be represented by the contact forces $\mathbf{F}_1$ and $\mathbf{F}_2$, which by the Newton’s third law satisfy the following relation:

$$\mathbf{F}_1 = -\mathbf{F}_2$$  (4)

We take $\mathbf{F} = \mathbf{F}_1$ and decompose $\mathbf{F}$ into the normal and tangential components, $\mathbf{F}_n$ and $\mathbf{F}_T$, respectively as $\mathbf{F} = \mathbf{F}_n + \mathbf{F}_T = F_n \mathbf{n} + F_T \mathbf{T}$, where $\mathbf{n}$ is the unit vector normal to the particle surface at the contact point (Fig. 1a).

The value of the contact forces $F_n$ and $F_T$ is obtained using a constitutive model formulated for the contact between two rigid elements. The contact interface in our formulation is characterized by the normal and tangential stiffness $k_n$ and $k_T$, respectively, the Coulomb friction coefficient $\mu$, and the contact damping coefficient $c_n$ (Fig. 1b). For details see [5, 8, 9].
3 FINITE ELEMENT FORMULATION

In the present work the so-called explicit dynamic formulation of the finite element equations of structural dynamics is used. The discretized equations of motion in the current configuration have the following form:

$$ M_F \ddot{r}_F = F_{\text{ext}}^F - F_{\text{int}}^F , $$

(5)

where $M_F$ is the mass matrix, $r_F$ is the vector of nodal displacements in the finite element mesh, $F_{\text{ext}}^F$ and $F_{\text{int}}^F$ are the vectors of external loads and internal forces, respectively. The global matrices and vectors, $M_F$, $F_{\text{ext}}^F$ and $F_{\text{int}}^F$, are assembled from the respective elemental matrices and vectors, $m_e$, $f_{\text{ext}}^e$ and $f_{\text{int}}^e$, defined as follows:

$$ m_e = \int_{\Omega_e} \rho N^T N \, d\Omega_e , \quad f_{\text{int}}^e = \int_{\Omega_e} B^T \sigma \, d\Omega_e , \quad f_{\text{ext}}^e = \int_{\Omega_e} N^T \rho b \, d\Omega_e + \int_{\Gamma_e} N^T t \, d\Gamma_e $$

(6)

where $\rho$ is the mass density, $\sigma$ is the Cauchy stress tensor, $b$ are the body forces, $t$ is the surface traction, $N$ is the matrix of interpolation (shape) functions and $B$ is the linear strain-displacement operator matrix [8].

Similarly to the DEM algorithm (Equation (2)), the central difference scheme is used for time integration of Equation (5):

$$ \ddot{u}_F^n = M_F^{-1} (F_{\text{ext}}^F - F_{\text{int}}^F)^n , \quad \dot{u}_F^{n+1/2} = \dot{u}_F^{n-1/2} + \ddot{u}_F^n \Delta t , \quad u_F^{n+1} = u_F^n + \dot{u}_F^{n+1/2} \Delta t . $$

(7)

Use of a diagonalized mass matrix yields a decoupled set of equations, and eliminates the necessity of matrix inversion in Equation (7.1). This leads to a very efficient solution for each time step. For details see [5, 8, 9].

4 COMBINED DEM/FEM MODEL

The coupling of DEM and FEM techniques leads to a powerful scheme for analysis of multifracture problems in solids. Successful attempts to develop a coupled DEM/FEM algorithm have been reported in [5, 4]. The adaptive DEM/FEM multiscale model used in this work is obtained by combining the discrete element and finite element methods in different subdomains of the same body. The coupling algorithm used here follows the concept presented in [10] for molecular dynamics coupling with a continuous model. The DEM and FEM subdomains can overlap each other. In this way a transitory zone between the microscopic-scale zone (discrete elements) and the macroscopic-scale zone (finite elements) is introduced. In the overlapping zone contributions of each of the two methods to the overall stiffness vary gradually. This allows us to avoid or minimize unrealistic wave reflections at the interface between the DEM and FEM domains.

The total domain $\Omega$ is split into two subdomains: $\Omega_F$, discretized with finite elements and $\Omega_D$, modelled with discrete elements. Domains $\Omega_F$ and $\Omega_D$ can overlap with each
other over a region $\Omega_{DF}$ (Fig. 2). The virtual work (VW) in the total domain $\Omega$ ($\delta W_\Omega$) is written as a linear combination of the virtual work in the subdomains $\Omega_F$ and $\Omega_D$, i.e.

$$\delta W_\Omega = \alpha \delta W_F = (1 - \alpha) \delta W_D$$

where $\alpha$ is a parameter that takes a zero value on $\Omega_D$, a unit value on $\Omega_F$ and it varies linearly between 0 and 1 on the overlapping region $\Omega_{D-F}$.

Subdomains $\Omega_F$ and $\Omega_D$ are coupled in the overlapping region $\Omega_{D-F}$. Coupling is introduced via kinematic constraints relating the displacements ($u$), velocities ($\dot{u}$) and accelerations ($\ddot{u}$) of the nodes of the finite element mesh and the discrete elements belonging to $\Omega_{D-F}$. The kinematic constraint can be generically written as

$$\delta u_{Di} - N_F \delta u_F = 0 \; , \; \dot{u}_{Di} - N_F \dot{u}_F = 0 \; , \; \ddot{u}_{Di} - N_F \ddot{u}_F = 0$$

where ($\cdot)_D$ and ($\cdot)_F$ respectively denote values at the discrete element $i$ and the finite element mesh nodes and $N_F$ are the standard FEM shape functions. The constraints (9) are applied on the overlapping region $\Omega_{D-F}$ only.

The constraints (9) are introduced in the VW equation via a penalty function method. For details see [9].

5 ADAPTIVE DEM-FEM SCHEME

An adaptive DEM/FEM solution procedure has been developed based on the progressive introduction of discrete elements in zones of the finite element mesh where cracking and multifracture occurs. This optimizes the use of discrete elements to zones where they can be more effective which considerably simplifies the contact search process.

In essence, the adaptive DEM/FEM procedure operates as follows:

1. Start with a discretization of the analysis domain using a finite element mesh only (i.e. $^o\Omega \equiv ^o\Omega_F$).

2. At each time instant ($t$) check the stress and strain levels at each element. For linear triangles and tetrahedra this simple implies computing the strains and stresses at the element centroid.
3. Evaluate the threshold of failure (fracture) of each element. This can be done via procedures based on the point-wise value of the stresses (or the strains), or using an adequate energy norm. In our work a simple Tresca failure model has been used to define the onset of fracture at the element mid-point.

4. Introduce a collection of discrete elements within the finite elements that have exceeded the failure threshold. In our work this occurs when the stresses at the element mid-point reach 90% of the Tresca failure stress. At this moment, the continuum region previously occupied by finite elements is now modelled with a collection of discrete elements.

The introduction of discrete elements will create an overlapping between the new discrete elements and the finite elements remaining in the mesh. Overlap DEM/FEM regions are treated as explained in the previous section.

5. Solve for the displacements, velocities and accelerations of the regions occupied with finite elements ($\Omega_F$) and discrete elements ($\Omega_D$) at $t + \Delta t$ using the explicit schemes (2) and (7) with the constraints (9).

6. The introduction of additional discrete element regions on the finite element mesh evolves in time in an adaptive manner accordingly to the evolution of the stress and strain fields in the analysis domain.

For blast problems the transition of the finite element mesh to the discrete element region occurs quite rapidly, as the fracture zone progresses almost at the blast speed on the whole analysis domain. However, the adaptive DEM/FEM procedure is still effective in these cases as the time increment for the explicit solution is very small and the delay in introducing discrete elements leads to considerable savings in computing time.

6 EXAMPLES

6.1 Failure of a vertical wall due to blast loading

This relatively simple 2D example shows the failure of a vertical masonry wall induced by a blast loading due to an explosive placed within a concrete box modelled with discrete elements (Fig. 3a). The effect of the explosive is simulated by an impulse pressure load, with a peak pressure of 600 MPa acting the center of the box. The explosion induces the multifracture of the box in many fragments that impact the adjacent wall inducing its instant failure (Fig. 4).

The cylinder wall has been initially discretized with a mesh of finite elements. The discrete elements have been progressively introduced in the wall using the adaptive DEM/FEM coupling algorithm. The evolution of the discrete element region in the wall is shown for three time instants in Figure 5.

Figure 6 shows a similar 2D problem for a masonry tunnel under the same type of blast loading.
6.2 Analysis of the fracture of a double curvature dam due to blast loading

The final example is the study of the fracture induced by a blast load on a double curvature concrete dam. The load is induced by an explosive placed at the top of the central section, reproducing the effect of the explosion of a vehicle circulating over the dam top. The region adjacent to the explosion has been modelled with discrete (spherical) elements while the rest of the dam has been modelled with standard 4-noded tetrahedral elements.

Figure 7 shows the evolution of the fracture at the dam top due to the explosion and the final fractured zone.
Eugenio Oñate, Carlos Labra, Francisco Zarate and Jerzy Rojek

Figure 6: Masonry cylinder under internal blast load induced by an explosive within a concrete box. Deformation of structure at three time instants.

Figure 7: Effect of a blast load an a double curvature dam. The explosive load has been modelled as a peak pressure load of 600 MPa acting at the center of the dam top.

7 CONCLUDING REMARKS

The adaptive DEM/FEM procedure presented in this work is an effective technique for the modelling and simulation of the progressive multi-fracture and failure of structures
due to blast loading. The adaptive DEM/FEM scheme allows the optimal use of DEM and FEM in different parts of the structure as the failure region evolves.

REFERENCES


STRATEGIES FOR SIMULATION SOFTWARE QUALITY ASSURANCE APPLIED TO OPEN SOURCE DEM - PARTICLES 2011

Stefan AMBERGER*, Christoph GONIVA*, Alice HAGER*, Christoph KLOSS*

*Christian Doppler Laboratory on Particulate Flow Modelling
Johannes Kepler University
Altenbergerstr. 69, 4020 Linz, Austria
e-mail: stefan.amberger@cfdem.com, www.cfdem.com

Key words: Granular Materials, Open Source DEM, Quality Assurance, Test Harness

Abstract. We present a strategy to improve the software quality for scientific simulation software, applied to the open source DEM code LIGGGHTS [1] [2]. We aim to improve the quality of the LIGGGHTS DEM code by two measures:

Firstly, making the simulation code open source gives the whole user community the possibility to detect bugs in the source code and make suggestions to improve the code quality.

Secondly, we apply a test harness, which is an important part of the work-flow for quality assurance in software engineering [5]. In the case of scientific simulation software, it consists of a set of simulation examples that should span the range of applicability of the software as good as possible. Technically, in our case it consists of a set of 10-50 LIGGGHTS simulations and is being run automatically on our cluster, where the number of processors, the code features and the numerical models are varied. Qualitative results are automatically extracted and are plotted for comparison, so thus a huge parameter space of flow regimes, numerical models, code features and parallelization situations can be governed.

A test harness can aid in (a) finding bugs in the software, (b) checking parallel efficiency and consistency, (c) comparing different numerical models, and, most importantly, (d) experimental validation. Parallel consistency means that within a parallel framework, we need to have the possibility to compare the answers that a run with a different number of processors gives and the time that it takes to compute them. Experimental validation is especially important for scientific simulations. If experimental data is available for a test case, the experimental data is automatically compared to the numerical results, by means of global quantities such number of particles in the simulation, translational and rotational kinetic energy, thermal energy etc.
The LIGGGHTS test harness aims to be a transparent and open community effort that everybody can contribute to in order to improve the quality of the LIGGGHTS code. We illustrate the usefulness of the test harness with several examples, where we especially focus on experimental validation.

1 INTRODUCTION

This paper presents one instance of testing as a possible strategy for software quality assurance, using the example of the test harness, that is used for LIGGGHTS development.

Reading instructions for this paper are the following: The chapter Classification shows the main reason why we used testing as the strategy of our choice. Following that the chapter Functional Range presents the functionality of our test harness. The structure of our test harness and terminology (names of modules) we use later on are defined in section Basic Structure of the Program. At last we present several examples in order to emphasize the benefits of highly modular software in section Examples and afterwards conclude the paper.

2 CLASSIFICATION

One can distinguish two types of software verification: static verification and dynamic verification.

For large systems like LIGGGHTS static verification, especially non-heuristic methods, i.e. methods capable of actually proving the correctness of software by means of formal methods of mathematics via automated theorem provers, are topic of current research and not yet applicable [4]. A more applicable approach used excessively by software developers is dynamic verification alias testing. One main purpose of this test harness is to do large scale system tests on user defined sets of inputs, automatically verifying the correctness of the output via comparison with the output of previous versions of LIGGGHTS as well as data obtained via experiments, thus guaranteeing version consistency.

3 FUNCTIONAL RANGE

The design of this test harness allows it to be used to

1. assure version consistency
2. detect bugs in newly added functionality
3. detect and pinpoint bugs accidentally introduced while updating
4. detect unwanted behaviour of newly implemented models
5. check parallel efficiency and consistency
6. compare different numerical models (w.r.t. cpu time, total translational / rotational kinetic energy of the simulated system)

7. provide a platform for generating sets of data for experimental verification

8. automated and repeated model verification via experimental data

4 BASIC STRUCTURE OF THE PROGRAM

The test harness consists of four main parts that can be combined in different ways to yield different results, thus supporting a wide range of application (see section 3).

In step one a folder structure is generated: for each executable (one or two) a folder containing all examples and all input-scripts is created. These input-scripts are then sequentially simulated with the respective executables. All this happens on the cluster, where multiple nodes can be accessed by LIGGGHTS via MPI, according to what the input-scripts of the respective examples require. The output of each simulation is stored in a folder which unique name indicates success, failure or abortion of the simulation. Figure 1 shows a typical folder-structure created by step1, where “in_n.ex” is the n-th input-script of example ex and nameof_executable1 / nameof_executable2 are the (file)names of the executables used. The name of this step is step1.

In step two the test harness branches: depending on which data was produced in step one (dump-data: coordinates, velocities, and radii of all particles for each timestep OR thermo-data: timestep, number of particles, translational and rotational kinetic energy of the system, cpu-time) one chooses the branch accordingly. In this phase two data sets

![Figure 1: Typical folder structure created by step1](image)
in the form of folder structures of step one are compared. This happens in 5 (6) steps in step2_dump (and step2_thermo):

1. For all examples it is checked whether the simulation finished successfully.
2. For all examples which successfully finished the number of timesteps is checked (or difference thereof).
3. For all examples that passed tests one and two positively and without differences the normalized (regarding total number of particles) root mean square of the number of particles per timestep is calculated.
4. and 5. For all examples that passed tests one and two positively and without differences the normalized (regarding total number of particles and total translational / kinetic energies) root mean square of translational and rotational kinetic energies are calculated.
5. the difference in CPU time is calculated. This only happens with thermo output.

This step outputs a table that shows the differences between the two simulations of corresponding examples on different executables and basic properties of the simulation. If the folder-structure, that is analyzed during execution of the step, contains only the output of one executable the program automatically tries to extract basic properties of the simulation instead of comparing to data of another simulation. The name of this steps are step2_dump and step2_thermo.

The third part of the test harness is software, that parses input-scripts of LIGGGHTS and detects differences therein, thus allowing to locate bugs if some scripts fail to execute, and some do not. The output of this part is a table showing which LIGGGHTS functionality is called during execution, allowing easy comparison of input-scripts. The name of this part of the program is compareIS.

The fourth part of the test harness allows to compare experimental data e.g. in the sense of hopper mass-flow rate [3] to data obtained by simulations, and prints a visualization of the accuracy of the models used. The name of this part is mDischarge.

These four parts can be combined in different ways to yield different results. Some of the possible combinations are listed in section 3 and described in section 5.

5 EXAMPLES

5.1 Assuring Version Consistency

After simulating three examples with step1 the algorithm outputs a folder structure similar to Figure 1. This structure now can be the input of step2_dump. This yields output like illustrated in Figure 2. In this example one can easily see, that both translational and rotational kinetic energy changed slightly in one example (ex3). This - if not willingly introduced - indicates inconsistencies between the two versions of this test.
5.2 Detecting Bugs in Newly Added Functionality

Via running a relatively large number of examples one can check whether some new functionality has obvious errors or not. *Step1* can run the simulations (also on only one executable, namely the newly compiled one), which results can be interpreted with *step2_dump* or *step2_thermo* respectively. For now we assume the set of simulations suitable for testing the newly added functionality output dump data. Then *step2_thermo* outputs a *.csv* like in Figure 3. Here the following examples did not finish, thus resulted in abortion due to a bug: example 1: input-script 1, example 3, example 5, example 6: input-script 1 and example 8: input-script 2. If one knows properties of these examples that differentiate them to the examples that finished the simulation one knows where to search for the bug. Also *compareIS* can now be used to pinpoint the function that causes the termination of the simulation.

5.3 Detecting and Pinpointing Bugs Accidentally Introduced While Updating

Detecting Bugs can be done like in Subsection 5.1. Now assume we have three input-scripts, two of them work perfectly fine and one (the third one) not functioning properly. *compareIS* returns a table that shows the used functionality of LIGGGHTS of the respective input-scripts and might look like the one in Figure 4, suggesting an error related to either the command *processors* or the command *pair_style.*
5.4 Checking Parallel Efficiency

For checking parallel efficiency a set of examples can be run two times, using a different number of processors. The number of processors is changed automatically. The output of both simulations afterwards is combined into one folder, simulating the output of step1. This time however this folder does not, as usual, contain the output of two different executables, but the output of one executable but using a different number of processors in each simulation. Hence step2 thermo compares these runs and shows the speedup in the last column of the output-table. Figure 5 shows one possible output, run for examples ex1, ex2 and ex3. In this figure all examples have about the same speedup, due to the small problem size only about 1.6.

5.5 Experimental Validation via Hopper Mass Flow Rate

One way of verifying the models used is to measure the hopper mass flow rate of e.g. glass beads and compare the results to the hopper mass flow rate of a corresponding simulation that models the experiment. A concrete example incorporated 28 experimental setups, using mono-disperse spherical glass beads of particle diameters ranging from 2-4 mm and variable hopper orifice diameters, ranging from 14-38 mm. The hopper that was used was equivalent to the hopper described by Kloss, Goniva and Pirker [2]. A simulation snapshot can be seen in Figure 6(a), the results in Figure 6(b). For most of the cases the simulated and measured mass flow rates were in good agreement.
6 CONCLUSION

It is vital to assure consistency and accuracy of models, thus the developers of LIGGGHTS put high emphasis on testing and verifying. In this context the modularity of this test harness allows it to be used in a wide area of applications and makes quality assurance easier and faster.

REFERENCES


ADVANCES IN THE PARTICLE FINITE ELEMENT METHOD FOR FSI: A MODIFIED FRACTIONAL STEP APPROACH

PAVEL RYZHAKOV*, EUGENIO OÑATE*, RICCARDO ROSSI* AND SERGIO IDELSOHN†

*Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE)
Universitat Politècnica de Catalunya
Campus Norte UPC, 08034 Barcelona, Spain
e-mail: pryzhakov@cimne.upc.edu, www.cimne.com/

†ICREA Research Professor at CIMNE

Key words: fluid-structure interaction, FSI, PFEM, Lagrangian fluids, fractional step, penalty

Abstract. The Particle Finite Element Method was originally developed for applications involving incompressible fluids containing free surfaces. The PFEM’s fundamental features include a) updated Lagrangian description b) nodal storage of variables, c) re-meshing, d) alpha-shape based free surface determination. Several fluid formulations sharing these basic ideas of the PFEM [1] have been developed over the past decade. One can classify the existing PFEM fluid formulations into 2 main groups: purely incompressible and quasi-incompressible ones. It was found that the quasi-incompressible formulations led to a number of advantages when applied to FSI problems involving flexible structures. However, in these latter formulations, the desired incompressible solution was only approximated and numerical difficulties when approaching the incompressibility limit (i.e. using very large values of the compressibility constant) were faced.

In the present work we introduce the PFEM formulation of the new generation: it combines the best features of the previously developed methods and leads to incompressible solution, while preserving some features of the quasi-incompressible formulations advantageous for the FSI.

1 INTRODUCTION

The Particle Finite Element Method (PFEM) was originally developed for solving problems involving gravitational incompressible flows containing free surfaces and was found to be advantageous for the fluid-structure interaction (FSI) [1]. Several fluid formul-
olutions/strategies have been utilized within the overall framework of the PFEM over the past years.

Fractional step method is possibly the most widely used approach for solving the incompressible Navier-Stokes equations due to the efficiency gained by decoupling velocity and pressure variables. The first works on the Particle Finite Element Method (PFEM) utilized pressure segregation via fractional step [1]. On the other hand, penalty and related quasi-incompressible methods define another competitive option and lead to certain advantages. In particular, it was shown that for the solution of fluid-structure interaction (FSI) problems, introducing the slight compressibility into the fluid leads to significant advantages for the FSI[3], [2]. One may naturally define a monolithic FSI solver, permitting to treat cases (such as interaction with light-weight structure) where many other approaches fail. While leading to efficient FSI strategies, a certain number of drawbacks was associated to the quasi-incompressible methods: a) poor pressure stability for high values of the compressibility constant (incompressible limit) b) the solution only approximates the true incompressible solution.

In the present work we propose a methodology that combines the ideas of the previous works. We strive to develop a truely incompressible formulation, while preserving the features of quasi-incompressible approaches advantageous for coupling with the structure in FSI. This is achieved by modifying the pressure term in the fractional momentum equation. The idea is to use a prediction upon the end-of-step pressure. The objective is to use such an approximation that should not involve resolution of any equations system, thus not increasing the computational effort considerably. Including the approximated end-of-step pressure (instead of the previous step pressure) in the fractional momentum equation results in an intermediate velocity being much closer to the end-of-step velocity, than in a standard fractional step procedure. Thus, the convection can be resolved much better.

As in the classical fractional step method, once the fractional velocity is computed, the Poisson’s equation is solved for the pressure. The Poisson’ equation in our technique serves as a corrector acting upon the predicted pressure field to give the final incompressible end-of-step pressure. Having computed the end-of-step pressure, the correction step is applied in a standard manner and the incompressible velocity end-of-step velocity is obtained.

2 MODIFIED FRACTIONAL STEP

The discrete momentum-continuity system (for simplicity we use BE scheme for the illustration; the details upon the space discretization are omitted) for the incompressible flow in the updated Lagrangian framework can be written as:

\[ \mathbf{r}_m = \mathbf{F} - \left( \rho \mathbf{M} \frac{\mathbf{v}_{n+1} - \mathbf{v}_n}{\Delta t} + \mu \mathbf{L} \mathbf{v}_{n+1} + \mathbf{G} \tilde{p}_{n+1} \right) \]  

(1)

\[ \mathbf{D} \mathbf{v}_{n+1} = 0 \]  

(2)
where \( r_m \) is the momentum equation residual\(^1\), \( M \) is the mass matrix, \( L \) is the Laplacian matrix, \( G \) is the gradient matrix, \( \tilde{v}, \tilde{p} \) and \( \mu \) are the velocity, pressure and viscosity respectively and \( F \) is the body force vector.

Next we introduce the modified fractional step split, that consists in using a pressure prediction in the fractional momentum equation:

\[
\tilde{r}_m = F - \left( \rho M \frac{\tilde{v} - \tilde{v}_n}{\Delta t} + \mu L \tilde{v} + G \tilde{p}_{n+1}^g \right) \tag{3}
\]

\[
\rho M \frac{\tilde{v}_{n+1} - \tilde{v}}{\Delta t} + G (\tilde{p}_{n+1} - \tilde{p}_{n+1}^g) = 0 \tag{4}
\]

\[
D \tilde{v}_{n+1} = 0 \tag{5}
\]

The pressure Poisson equation is obtained by applying the incompressibility condition \(^5\) to the end-of-step momentum equation, leading to

\[
D \tilde{v} = \Delta t DM^{-1} G (\tilde{p}_{n+1} - \tilde{p}_{n+1}^g) \tag{6}
\]

For simplicial equal interpolation order mixed elements, pressure needs to be stabilized. This consists in adding a stabilization term into the pressure equation. Indicating the stabilization term (we do not specify here the particular stabilization technique) as \( \tau S \) and using the approximation \( DM^{-1} G \approx L \), we arrive at the final system:

\[
\tilde{r}_{mom} = F - \left( M \frac{\tilde{v} - \tilde{v}_n}{\Delta t} + \mu L \tilde{v} + G \tilde{p}_{n+1}^g \right) \tag{7}
\]

\[
D \tilde{v} = \Delta t L (\tilde{p}_{n+1} - \tilde{p}_{n+1}^g) + \tau S \tilde{p}_{n+1} \tag{8}
\]

\[
M \frac{\tilde{v}_{n+1} - \tilde{v}}{\Delta t} + G (\tilde{p}_{n+1} - \tilde{p}_{n+1}^g) = 0 \tag{9}
\]

**Fractional momentum equation solution** To solve the fractional momentum equation, the pressure prediction \( \tilde{p}^g \) shall be computed. Note that assuming that it is equal to zero \( (\tilde{p}^g = 0) \) or to the previous step pressure \( (\tilde{p}^g = \tilde{p}_n) \) would recover standard first and second order fractional step schemes respectively. In this work we propose to obtain the prediction by associating the pressure increment with the volume change as (this way of computing pressure is presented in detail in [3]), equivalent to assuming the slight compressibility.

\[
\delta \tilde{p}^I = \frac{\delta V^I}{V^I_n} \tag{10}
\]

where \( \tilde{p}^I \) is the pressure at the node \( I \), \( \kappa \) is the compressibility constant and \( V^I_n \) is the nodal volume (we associate to each node of the FE mesh a nodal volume defined in such

\(^1\)Note that writing the equations in the updated Lagrangian framework, i.e. in the unknown configuration \( x_{n+1} \), makes the discrete operators non-linear and obliges us to use residual form.
a way that it coincides with the diagonal entry of the diagonalized pressure mass matrix $ar{V}_I := M_{p,II}$.

Application of Newton’s method to the solution of the non-linear fractional momentum equation (Eq. 7) requires to evaluate the dynamic tangent matrix $H$:

$$H = \frac{\partial r_{frac}^m}{\partial v} = \frac{M}{\Delta t^2} + \mu L + \kappa GM^{-1}D$$

(11)

where the last term corresponds to the linearization of the pressure gradient (see [3]).

One can see, that the tangent of the fractional momentum equation contains the volumetric term, i.e. linearization of the pressure gradient. The additional computational cost due to the pressure update is minimal, as it does not involve solution of any system, provided that the unknown pressure is multiplied by the lumped pressure mass matrix. The cost of adding the $\kappa GM^{-1}D$ term to the tangent matrix can be minimized by using a matrix-free method (see [3]).

**Pressure Poisson’ equation and the correction step** The next step to be carried out is the correction of the pressure, i.e. obtaining the end-of-step incompressible pressure. This is done by solving Eq. 8. Solution of Eq. 8 requires to impose the pressure boundary condition. While usually zero pressure is fixed at the free surface, we propose to use a physically more meaningful option, i.e. the predicted pressure. The predicted “quasi-incompressible” pressure is a meaningful physical approximation, provided that the compressibility constant $\kappa$ used in the pressure prediction is large.

This step can be thus viewed as a correction of the predicted pressure $\bar{p}_{n+1}^p$ to the correct end-of-step one everywhere except for the free surface, where the predicted pressure is kept as a Dirichlet b.c..

The correction step is carried out according to Eq. 9 and returns the end-of-step divergence-free velocity.

### 3 FLUID-STRUCTURE INTERACTION

The method proposed can be easily implemented within monolithic FSI strategies proposed in our previous works [3], [2]. According to these approaches a unique discretization is applied to the entire domain, containing the fluid and the structure where a single monolithic FSI system of equations is solved. Thus the interaction becomes an intrinsic feature of the method and does not involve coupling iterations and boundary condition exchange between the fluid and the structure sub-domains. The fractional momentum equation for the fluid and the momentum equation of the structure are assembled into a single system of equations. This step completely coincides with the procedure proposed in [3], [2]. However, in former strategies the obtained velocity field was considered to be the end-of-step velocity, thus approximating the incompressible behavior by the slightly compressible one. In the present approach two further steps are carried out. The first one is the solution of the Poisson’s equation in the fluid domain. This allows the use conventional pressure
stabilization techniques and smooths the pressure field, which is particularly important when high values of the compressibility constant is used at the prediction step. This step affects exclusively the fluid domain. In order to maintain the strong coupling between the fluid and the structure it is important to modify the correction step. In order to obtain the end-of-step velocity, instead of the projection step (Eq. (9)) carried out exclusively for the fluid domain, we propose to re-solve the monolithic FSI momentum equation using the gradient of the newly obtained end-of-step pressure. The approach can be also applied in the partitioned context. There is some evidence that due to the presence of the predicted pressure in the fractional momentum equation, classical Dirichlet-Neumann (failing when standard fractional step approach is used) coupling may work.

4 EXAMPLE

This example tests the performance of the method in its application to a fluid-structure interaction problem. The benchmark is described in [4] and deals with a laminar flow over a fixed cylinder, with an elastic beam attached to it. The velocity field and horizontal and vertical displacements of the beam are analyzed. The chosen material properties correspond to the most challenging FSI setting: density ratio between the fluid and the structure is equal to 1.

Fig. 1 shows the velocity field at two time instances and Fig. 2 displays the comparison of the temporal evolution of vertical and horizontal displacements of point A (comparison with the results of [4]).

The results obtained in both test cases and their comparison with the results presented in [4] prove applicability of the method in the field of the FSI. Numerical tests have shown that already on coarse meshes the behavior of the flow and its interaction with the structure can be well-reproduced. In comparison with the classical fractional step method, the approach proposed here did not require any additional techniques in order
REFERENCES


APPLICATIONS OF THE PARTICLE FINITE ELEMENT METHOD IN DAM ENGINEERING

FERNANDO SALAZAR*, DANIEL POZÓ*, RAFAEL MORÁN** AND EUGENIO OÑATE*

*Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE)
Campus Norte UPC, 08034 Barcelona, Spain
e-mail: fsalazar@cimne.upc.edu, dpozo@cimne.upc.edu, onate@cimne.upc.edu, www.cimne.com

** UPM-CIMNE Classroom. ETSI Caminos, Canales y Puertos
Technical University of Madrid (UPM)
C/ Profesor Aranguren s/n, 28040 Madrid, Spain
e-mail: rmoran@caminos.upm.es, www.caminos.upm.es

Key words: PFEM, Reservoirs, Spillways, Aeration, Outlets, Landslides, Erosion, Hydraulics

Summary. The paper presents the results of the application of the Particle Finite Element Method (PFEM) to the analysis of some of the more complex phenomena related to dam hydraulics: shock waves in spillways, aeration in bottom outlets, and erosion in the downstream river bed. Furthermore, the method has been applied to the study of the consequences of landslides in reservoirs: the wave generation, its propagation, and the affection to the dam.

1 INTRODUCTION

In the recent years, a great effort has been made in the International Center for Numerical Methods in Engineering in the development and implementation of the Particle Finite Element Method [1]. As a result, its application to a wide number of engineering problems is possible, such as fluid dynamics, fluid-structure-interaction, and erosion, among others [2]. CIMNE-Madrid group focuses in research into the field of dam safety, and has taken advantage of PFEM capabilities to analyze some of these phenomena. The paper briefly describes four examples of the application of PFEM to different problems related to dam hydraulics and dam safety: a) shock waves in spillways, b) aeration in bottom outlets, c) erosion, and d) landslides in reservoirs.

In our days, the most frequently used methodology for designing a hydraulic structure follows four steps: a) preliminary design based in experience and experimentally based manuals, b) laboratory tests campaign of this design to check its performance, c) modifications to the original design on the basis of the results of the tests, and d) construction of the final design.

Different numerical tools, some of them commercially available, have shown their capability to model most of the hydraulic problems to be considered in dams. Some of them use Eulerian formulations, and some others use a fully Lagrangian approach.
In spite of that, numerical modeling is rarely used in this process, unlike other kind of calculations, such as structural design, where numerical methods have displaced experimental tests almost completely.

Furthermore, there are still several challenges to be solved in the field of dam hydraulics. Some of the most relevant are related to the consideration of air-water interaction in bottom outlets and spillway chutes. This topic is very hard to analyze through physical testing due to scale effects and reliability of data acquisition, although it is of great importance in most structures subjected to supercritical flows. Numerical modeling seems to be an appropriate tool to assess this problem.

PFEM uses a Lagrangian approach combined with the resolution of the equations via the Finite Element Method (FEM). In order to do that, a finite element mesh has to be generated, which is typically updated every time step. With this strategy, the convection of the nodes can be reproduced accurately, while imposing Dirichlet conditions in a natural way. A detailed description of the method is not the objective of the paper, but the reader can find it in [1, 2] PFEM has been validated to reproduce some of the above mentioned hydraulic problems [3].

2 SHOCK WAVES IN SPILLWAY CHUTES: ITOIZ DAM CASE STUDY

PFEM has proven to be appropriate for the simulation of hydraulic problems in which the free surface is irregular, and greatly changes in shape during the transient solution. There are several examples in the literature, some of which have been used as benchmark problems, such as the typical dambreak example. The previous results [3] suggest that PFEM could be a useful tool in the hydraulic calculation of spillway chutes in which shock waves are expected.

Itoiz Dam is one of the most popular and recent structures constructed in Spain having a converging chute in its service spillway due to the lack of space in the downstream toe of the dam. The chute width varies from 53.75 m in the crest to 22.70 m at the entrance of the stilling basin. Figure 1a shows a picture of the dam, while figure 1b contains a view of the geometry of the numerical model. Some of the most relevant features of the spillway are included in Table 1.

<table>
<thead>
<tr>
<th>Table 1: Characteristics of Itoiz Dam spillway</th>
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<tbody>
<tr>
<td>Maximum dam height</td>
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<tr>
<td>Spillway crest</td>
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<tr>
<td>Design flood (10,000 years return period)</td>
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A pre-design of the spillway was developed before the construction, whose performance was tested in laboratory. The results showed that two shock waves appeared next to the walls, which became wider in the downstream direction, until they collided. They caused inadequate flow distribution at the end of the chute, with flow accumulation in the centre of the channel which penetrated in the stilling basin like a dart, favoring agitation in the latter. The inclination of the chute walls caused the overspill of a part of the flow.

On the basis of the results of these tests, the design was modified, so as to reduce the shock waves, as well as to improve the efficiency of the stilling basin. The curves which defined the chute walls were smoothed, and the length of the stilling basin was increased.
Figure 1: Itoiz Dam spillway. Left: downstream photo of the actual dam. Right: numerical model

The convergence of the chute walls still generated two shock waves next to the walls, but the flow distribution at the entrance of the stilling basin was more uniform. Overspill was avoided. The global behavior of the stilling basin was acceptable, with lower velocities at the entrance, and better energy dissipation.

Figure 2: Itoiz Dam spillway. Left: original geometry. Shock waves collide at the end of the chute. Right: Final design. The shock waves remain, but they don’t meet, thus flow distribution is better at the toe.
The aim of the numerical model was to reproduce the results of the laboratory tests, both for the original and final geometries. Figure 2 shows snapshots of the results of the numerical modeling, both for the original (left) and final (right) designs. Note that the above mentioned features of the spillway performance are reproduced.

3 AERATION IN BOTTOM OUTLETS

Bottom outlets are key elements to control the water surface elevation in reservoirs. Since the early twentieth century it has been found that an aeration system is necessary in the downstream side of the gate to achieve an appropriate performance of the structure. The system is typically placed downstream of the sealing device to prevent consequences due to the appearance of negative pressures. Otherwise, damages caused by cavitation and vibration are relatively frequent.

Due to the great difficulty to collect data or to study the phenomenon either in situ or in full scaled experimental facilities, the analysis has traditionally been carried out via laboratory tests in small-scale physical models. The results of these works have been used to develop empirical formulations for the calculation of the design air flow of the aeration system. Many authors have carried out this kind of studies, being the most commonly used the ones by Sharma [4], USACE [5] and Campell and Guyton [6]. However, the results of the different authors are divergent. Most of them analyze the situation in which a hydraulic jump is formed in the downstream conduit, but little information is available about free flow. Finally, most of them were developed from tests on rectangular conduits, which were the most popular in the last century. The design of the aeration system for a circular conduit (much more common nowadays) is usually made by means of the extrapolation of those criteria to the circular section. The great number of involved parameters and their wide variation make this methodology have its limitations.

In our work, PFEM has been used to assess this problem, in which the treatment of the interaction and mixing of two fluids (air and water) with very different physical characteristics is the greatest difficulty to be overcome.

Figure 4: Two snapshots of one of the runs. Left: Vectors representing velocities on a longitudinal section, where it can be seen the air flow into the conduit. Right: Particles (nodes of the mesh) of the fluid layer (air layer has been turned off).
The method is being applied to verify the performance of the new flat-seat circular-section valves, whose design is being developed by the Spanish company INHISA as an alternative to the traditional Bureau-Type. This work is being undertaken in the frame of VADIVAP project.

PFEM has turned out to be able to reproduce the velocity field both for the air and the water downstream the gate, as well as the interaction between both fluids. Figure 4 shows a snapshot of one of the calculations, in which it can be seen the air flowing through the air vent into the outlet.

Despite the air flow is the key variable, most of the authors have expressed their results in terms of the relation between $\beta$ and the water Froude number, being $\beta$ the ratio $Q_a/Q_w$, where $Q_a$ is the air flow and $Q_w$ the water flow.

Figure 5 shows the results obtained with PFEM, compared with those given by the experimental campaign and formulation developed by Sharma [4], which is the most commonly used. The latter represents a line joining the maximum air flow for every value of the Froude number. Note that the results of the laboratory experiments show an important dispersion from that line.

The numerical tests cover a small portion of the experimental campaign in free flow conditions, but the maximum values of $\beta$ match Sharma’s law as can be noted in figure 5.

![Figure 5](image.png)

**Figure 5:** Left: numerical results for 30 m (diamonds) and 50 m (triangles) of upstream water pressure, in comparison with the expression by Sharma (line). Right: Original chart by Sharma, where it can be seen that his expression covers the maximums, as well as the dispersion of his results.
Once the model has been validated in that way, it is being used to run numerical tests to obtain conclusions about the design of the aeration system and to analyze the influence of every parameter in the air flow. It has been found that there are several variables which greatly affect the phenomenon, such as: a) shape of the conduit, b) diameter and length of the air intake, c) gate opening, d) upstream pressure, e) length of the conduit downstream of the gate, and f) hydraulic conditions in the downstream side (free flow/submerged flow) g) distance between gate and aeration conduit. The high number of involved parameters explains the difficulty of applying empirical formulation.

![Figure 6: Mixture of air (grey) and water (blue) in the conduit (longitudinal cross section).](image)

3 EROSION

Erosion is another important concern in spillways, especially in tailwater pool technology, as well as in other many fields of engineering, particularly in river hydraulics. A formulation for erosion analysis has been implemented in PFEM [7].

The erosion model is based on the frictional work at the surface originated by the shear stress in the fluid. The resulting erosion model resembles Archard law [8, 9] typically used for modeling abrasive wear in surfaces under frictional contact conditions. The algorithm for modeling erosion at the fluid bed can be summarized as follows:

1. Computation of the resultant tangential stress induced by the fluid motion in every point of the bed surface.
2. Computation of the frictional work originated by the tangential stress.
3. The onset of erosion at a bed point occurs when the frictional work exceeds a critical threshold value defined empirically according to the properties of the bed material.
4. When the critical threshold is exceeded, the node is detached from the bed region and it is allowed to move within the fluid flow, i.e. it becomes a fluid node (but it conserves its density).
5. Sediment deposition can be modeled by an inverse process. Hence, a suspended node adjacent to the bed surface is assigned to the bed domain when its velocity decreases below a threshold value.
Figure 6: Modeling of bed erosion with the PFEM

Figure 7 shows some images of the application of PFEM to the study of erosion downstream the sky jump spillway of Barriga Dam (Spain).

Figure 7. Modeling of bed erosion in the downstream area of Barriga Dam spillway with the PFEM.

The model reproduces the behavior of the laboratory tests carried out for this spillway [10],
in which the flow undermined an area near the impact, whereas a part of the dragged material was deposited immediately downstream.

The authors are working in the development of practical criteria to establish the proper relation between the geotechnical information commonly used to characterize the river bed (granulometry, porosity, cohesion, etc.) and the parameters of the numerical model: a) erosion parameter and b) minimum velocity threshold.

4 LANDSLIDES IN RESERVOIRS

The analysis of the consequences of landslides in reservoirs is another application not directly related to dam hydraulics, but to dam safety. PFEM is particularly suited for modeling landslides, their impact into the still water in the reservoir, the wave generation, its propagation, and its affection to the dam as well as other structures sited in the shores.

Landslides in reservoirs have caused several dambreaks in history, as well as a large number of casualties. Although the frequency of occurrence of landslides is low, they are the third most important natural hazard in terms of casualties, after earthquakes and floods.

Landslides in reservoirs have a special interest, because variations in the water surface elevation (particularly rapid drawdowns) can foster their occurrence. The presence of a reservoir for a long time make the material in the slopes turn saturated, thus increasing their pore pressure and reducing effective stress. This unstabilization is partially compensated by the raise of total stress provoked by the hydrostatic pressure of the water in the reservoir. A rapid drawdown eliminates this stabilization in a lapse which in general is too short to allow the pore pressure to dissipate, thus increasing the probability of occurrence of a landslide.

PFEM has been validated for its application in the simulation of the interaction between landslides and a still mass of water, which can be a reservoir, a bay or a lake [11]. Various benchmark tests have been carried out, in which the falling mass has been considered either as a rigid solid or as a viscous fluid with a high density.

Figure 8 shows the results of the simulation of the experiment carried out by Sælevik [12]. It consists of a group of prismatic boxes accelerated into a mass of water in a rectangular channel. Three sensors measured the evolution of the water surface elevation.

![Figure 8. Modeling of the experiment by Sælevik et al [12] with the PFEM. Left: Comparative snapshots between numerical and experimental tests in the wave generation stage. Right: Comparison of the evolution of the water surface elevation in the sensors (dotted line represents the results by PFEM, whereas solid line shows the experimental results).](image)
The model has been applied to the analysis of the Lituya Bay landslide, which is one of the most famous and well documented accidents of this kind. The landslide was originated by an earthquake and mobilized 90 million tons of rocks that fell on the bay originating a large wave that reached a height on the opposed slope of 524 m.

Figure 9 shows images of the simulation of the landslide with PFEM. The sliding mass has been modeled as a continuum with a prescribed shear modulus.

No frictional effect between the sliding mass and the underneath soil has been considered. Also the analysis has not taken into account the erosion and dragging of soil material induced by the landslide mass during motion.

PFEM results have been compared in terms of the maximum run-up in both northern and southern shores of the bay. In the first, the maximum run-up obtained with PFEM was 551 m (see figures 10 and 11), which is 5% higher than the value of 524 m. observed experimental by [13]. The maximum height location differs in 300 mts from the observed value [13]. In the southern shore the maximum water height observed was 208 mts, while the PFEM result (not shown here) was 195 m (6% error).

More information on the PFEM solutions of this example can be found in [11].

![Figure 9](image.png)

**Figure 9.** Lituya Bay landslide. Left: Geometry for the simulation. Right: Landslide direction and maximum run-up [11,13]

![Figure 10](image.png)

**Figure 10.** Simulation of Lituya Bay landslide with the PFEM. Wave generation stage.
5 CONCLUSIONS

PFEM has been applied to the simulation of different important phenomena related to dam hydraulics and dam safety. It has been found that its application can be useful both in the design stage, as a complement to experimental tests, and in the analysis of dam safety in front of landslides.

6 ACKNOWLEDGEMENTS

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Figure 11. Simulation of Lituya Bay landslide with the PFEM. Wave propagation and maximum run-up in the northern shore.
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6 REFERENCES

SMOOTHED PARTICLE HYDRODYNAMICS MODELING OF HYDRAULIC JUMPS

PATRICK JONSSON*, PÄR JONSÉN†, PATRIK ANDREASSON*, T. STAFFAN LUNDSTRÖM* AND J. GUNNAR I. HELLSTRÖM*

* Division of Fluid and Experimental Mechanics
Luleå University of Technology (LTU)
SE-971 87, Luleå, Sweden
e-mail: patrick.jonsson@ltu.se, www.ltu.se

† Division of Mechanics of Solid Materials
Luleå University of Technology (LTU)
SE-971 87, Luleå, Sweden
e-mail: par.jonsen@ltu.se, www.ltu.se

Key words: hydraulic jump, smoothed particle hydrodynamics, sph, particle study.

Abstract. This study focus on Smoothed Particle Hydrodynamics (SPH) modeling of two-dimensional hydraulic jumps in horizontal open channel flows. Insights to the complex dynamics of hydraulic jumps in a generalized test case serves as a knowledgebase for real world applications such as spillway channel flows in hydropower systems. In spillways, the strong energy dissipative mechanism associated with hydraulic jumps is a utilized feature to reduce negative effects of erosion to spillway channel banks and in the old river bed.

The SPH-method with its mesh-free Lagrangian formulation and adaptive nature results in a method that handles extremely large deformations and numerous publications using the SPH-method for free-surface flow computations can be found in the literature.

Hence, the main objectives with this work are to explore the SPH-methods capabilities to accurately capture the main features of a hydraulic jump and to investigate the influence of the number of particles that represent the system.

The geometrical setup consists of an inlet which discharges to a horizontal plane with an attached weir close to the outlet. To investigate the influence of the number of particles that represents the system, three initial interparticle distances were studied, coarse, mid and fine.

For all cases it is shown that the SPH-method accurately captures the main features of a hydraulic jump such as the transition between supercritical- and subcritical flow and the dynamics of the highly turbulent roller and the air entrapment process. The latter was captured even though a single phase was modeled only. Comparison of theoretically derived values and numerical results show good agreement for the coarse and mid cases. However, the fine case show oscillating tendencies which might be due to inherent numerical instabilities of the SPH-method or it might show a more physically correct solution. Further validation with experimental results is needed to clarify these issues.
1 INTRODUCTION

The main components of a large scale hydropower station are a large reservoir dam where rain and melt water is stored and the turbine/generator assembly which converts the potential energy stored in the water into electricity. The hydropower sector contributes to almost half of the total power production in Sweden. However, the overall contribution from the hydropower sector varies throughout the year due to variation in energy demand from the consumers which in turn is due to seasonal variation in temperature and maintenance shutdown of industrial processes. As production varies throughout the year and the amount of precipitation is uncontrollable the need to find ways to handle the water head in the reservoir is crucial to obtain optimal working conditions. If the inherent flow regulation by generation is insufficient, spillways are engaged. When spillways are used the potential energy of the water is converted to kinetic energy potentially causing erosion problems to structures in the spillway channel as well as in other water-ways downstream the spillway like old river beds. An effective way to reduce the high kinetic energy levels is to design the spillway channels to trigger a hydraulic jump which is a natural occurring phenomenon in free flowing fluids characterized by large energy dissipation mechanisms. The main feature of a hydraulic jump is a sudden transition of shallow and fast moving flow into a relatively slow moving flow with rise of the fluid surface to keep continuity. The transition phase is known as the roller where the free surface is highly disturbed and air entrapment occurs.

Modeling of highly disturbed free surface flows such as the hydraulic jump is complex when grid based method is used. Severe problems with mesh entanglement and determination of the free surface have been encountered. Meshfree methods such as the Smooth Particle Hydrodynamic (SPH) method have been shown to be a good alternative to grid based methods to overcome the above stated problems. The SPH-method has matured rapidly during the last decade or even years and was thus chosen as the computational method.

The aim with this work is thus to explore the capability of the SPH-methods to accurately capture the main features of a hydraulic jump and to investigate the influence of the number of particles that represent the system.

2 METHOD

2.1 Smoothed particle hydrodynamics

Smoothed Particle Hydrodynamics (SPH) is a meshfree, adaptive, Lagrangian particle method for modeling fluid flow. The technique was first invented independently by Lucy and Gingold and Monaghan in the late seventies to solve astrophysical problems in three-dimensional open space. Movement of astronomical particles resembles the motion of fluids, thus it can be modeled by the governing equations of classical Newtonian hydrodynamics. The method did not attract much consideration in the research community until the beginning of the 1990 when the method was successfully applied to other areas than astrophysics. Today, the SPH-method has matured even further and is applied in a wide range of fields such as solid mechanics (e.g. high velocity impact and granular flow problems) and fluid dynamics (e.g. free-surface flows, incompressible and compressible flows).

In the SPH-method, the fluid domain is represented by a set of non-connected particles which possess individual material properties such as mass, density, velocity, position and
Besides representing the problem domain and acting as information carriers the particles also act as the computational frame for the field function approximations. As the particles move with the fluid the material properties changes over time due to interaction with neighboring particles, hence making the technique a pure adaptive, mesh-free Lagrangian method. With adaptive is meant that at each time step the field approximation is done based on the local distribution of neighboring particles. The adaptive nature of the SPH-method together with the non-connectivity between the particles results in a method that is able to handle very large deformations as is the case for highly disordered free-surface flows such as hydraulic jumps.

To further clarify the methodology of the SPH-method, the following key steps is employed to reduce the partial differential equation (PDEs) governing the problem at hand to a set of ordinary differential equations (ODEs).

1. The problem domain is represented by a set of non-connected particles.
2. The integral representation method is used for field function approximation, known as the kernel approximation.
3. The kernel approximation is then further approximated using particles, i.e. the particle approximation. The particle approximation replaces the integral in the kernel approximation by summations over all neighboring particles in the so called support domain.
4. The summations or the particle approximation are performed at each time step, hence the adaptive nature of the SPH-method as particle position and the magnitude of the individual properties varies with time.
5. The particle approximation is employed to all terms of the field functions and reduces the PDEs to discretized ODEs with respect to time only.
6. The ODEs are solved using standard explicit integration algorithms.

A more detailed description of the methodology and the kernel- and particle approximations can be found in the textbook by Liu and Liu.\(^9\)

As concluded in previous work\(^{10,11}\) the SPH-method do not necessarily behave in the same manner as mesh-based computational methods where refinement of the mesh is anticipated to yield better solutions of the PDEs. Instead, further refinement or more particles in the SPH-method might lead to deterioration of solutions or even divergent behaviour. This may be caused by inherent numerical instabilities of the SPH-method.

### 2.2 Hydraulic jump

The main characteristic of a hydraulic jump is the sudden transition of rapid shallow flow to slow moving flow with rise of the fluid surface also known as a transition from supercritical to subcritical flow\(^3\). The transition is strongly dissipative which is favourable when energy should be consumed as when kinetic energy levels should be reduced in spillway flows. Further characteristics of hydraulic jumps is the development of a large-scale highly turbulent zone known as the “roller” with surface waves and spray, energy dissipation and air entrapment.
As stated above the hydraulic jump is characterized by a supercritical and a subcritical region where the depths are significantly different. These depths $d_1$ and $d_2$ are referred to as *conjugate depths* and can be seen in the schematic Figure 1.

**Figure 1:** Schematic figure of the hydraulic jump showing the conjugate depths $d_1$ and $d_2$ and the depth $d_3$ past the weir.

A dimensionless relation between the conjugate depths can easily be derived from continuity, momentum and energy equations for a rectangular channel by assuming hydrostatic pressure distribution and uniform velocity distribution at the up- and downstream end of the control volume. Furthermore, the friction between the bottom and the fluid and the slope of the bottom is both assumed to be zero. With these assumptions the conservation equations yield the dimensionless relation between the conjugate depths for a rectangular channel as,

$$
\frac{d_2}{d_1} = \frac{1}{2} \left( \frac{1 + 8Fr_1^2}{1 + 8Fr_1^2 - 1} \right)
$$

where $Fr_1$ is the upstream Froude number,

$$Fr_1 = \frac{v_1}{\sqrt{gd_1}}$$

which by definition must be greater than one. The upstream Froude number is also used as an indicator of the general characteristics of the jump in a rectangular horizontal channel as different upstream Froude numbers produce different types of hydraulic jumps.

Furthermore, the depth $d_3$ is derived in a similar manner with the same assumptions as above, further details can be found in the textbook by Chanson.
2.3 Numerical setup

To reduce the complexity of modeling a three-dimensional spillway channel with adherent hydraulic jump a two-dimensional, horizontal and single phase (water) model is studied here. Following previous work\textsuperscript{12,13} the material model MAT_NULL is used to model water with density $\rho = 1000 \text{ kg/m}^3$ and dynamic viscosity $\mu = 0.0015 \text{ Pa.s}$. The null material has no shear stiffness or yield strength and behaves in a fluid-like manner\textsuperscript{14}. As the dynamic viscosity $\mu$ is nonzero, a deviatoric viscous stress of the form,

$$\sigma_{ij} = \mu \varepsilon_{ij}^{\prime}$$

is computed where $\varepsilon_{ij}^{\prime}$ is the deviatoric strain rate\textsuperscript{15}. Furthermore, the null material must also be used together with an equation of state (EOS) defining the pressure in the material. Varas et al.\textsuperscript{13} used the Gruneisen equation of state which employs the cubic shock velocity-particle velocity, which also was used in this work. The wall boundaries were modeled as rigid shell finite elements and the interaction between the boundaries and the SPH-particles was governed by a penalty based node to surface contact-algorithm.

The geometrical setup of the problem can be seen in Figure 2 where the fluid enters the domain using the BOUNDARY_SPH_FLOW inlet condition with a prescribed inlet velocity of $v_1 = 1.5 \text{ m/s}$ and depth $d_1 = 0.02 \text{ m}$. The horizontal plane situated between the inlet and the weir measures 1.1 m and is prefilled to a depth equal to weir height, i.e. $d_1$. Both the prefill of the horizontal plane and the weir assembly was introduced to trigger the hydraulic jump faster. Furthermore, at 1.9 m downstream of the inlet the outlet is situated.

![Figure 2: Geometrical setup at $t = 0 \text{ s}$](image)

Initial results indicated that after an initial transient phase of roughly 3.0 s the hydraulic jump was fully developed. However, the roller region was non-stationary even after the initial transient phase and traveled upstream toward the gate with very low velocity, hence all subsequent simulation were run for five seconds to include such phenomena. Three different initial interparticle spacing $\Delta l (\Delta l = \Delta x = \Delta y)$ of 0.005 m (coarse), 0.004 m (mid), and 0.002 m (fine) were used to investigate the influence of the number of particles that represent the system. The total number of particles and the overall computational time for each case is summarized in Table 1.
Table 1: The total number of particles and the overall computational time for each case.

<table>
<thead>
<tr>
<th>Case</th>
<th>Total number of particles</th>
<th>Computational time [h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse ($\Delta l = 0.005m$)</td>
<td>6880</td>
<td>19 (12 cores)</td>
</tr>
<tr>
<td>Mid ($\Delta l = 0.004m$)</td>
<td>10750</td>
<td>29 (8 cores)</td>
</tr>
<tr>
<td>Fine ($\Delta l = 0.002m$)</td>
<td>43000</td>
<td>186 (12 cores)</td>
</tr>
</tbody>
</table>

All simulations were done using the commercial available software package LSCT LS-DYNA v. 971 R5.1.1 on HP Z600 Linux machines with eight to twelve cores.

3 RESULTS AND DISCUSSION

This part will start with a qualitative comparison of the three cases at successive time steps and end with a quantitative comparison of theoretically derived values and results from the simulations.

At $t = 0.0 \, s$ the fast incoming fluid begins to flow into the initially stationary fluid which starts to move together downstream, i.e. in the positive x-direction. A wave forms and breaks as more water flows onto the horizontal plane and at roughly $1.0 \, s$ it reaches the weir and starts to spill over. The fluid reaches the outlet at roughly $1.5 \, s$ and in the meantime the roller region has moved closer to the weir. The roller continues to move downstream towards the weir until roughly $3.0 \, s$ when the velocity of the roller declines rapidly and changes direction. Past $3.0 \, s$ a quasi-stationary state is attained as the velocity of roller upstream is very low. Figures 3-5 shows the three cases using the above stated number of particles with color coded velocities in the positive x-direction.
Figure 3: Visualization of the coarse ($\Delta l = 0.005 \, m$) case at successive time steps with color coded velocities in the positive x-direction.
Figure 4: Visualization of the mid ($\Delta l = 0.004 \text{ m}$) case at successive time steps with color coded velocities in the positive x-direction.
Figure 5: Visualization of the fine ($\Delta l = 0.002\, m$) case at successive time steps with color coded velocities in the positive $x$-direction.

Comparing the results in Figures 3-5 in a qualitative manner both the coarser cases produces smooth hydraulic jumps with well-defined free-surfaces especially past the roller region. The fine case behaves in a more chaotic manner with large oscillation of the free-surface which is clearly seen in the subcritical region past the roller. However, all three cases capture the main features of a hydraulic jump such as the high velocity small depth supercritical- and low velocity large depth subcritical region. Furthermore, the highly
turbulent roller where air entrapment occurs is clearly visible in all cases even though a single phase has been modeled only.

As stated above, the hydraulic jump is fully developed at roughly $3.0 \, \text{s}$ hence all data from the simulations was obtained past this time at intervals of $0.5 \, \text{s}$. In this work, the depth $d_2$ in the subcritical section and the depth $d_3$ in the contraction past the weir have been evaluated only. However, as can be seen in Figures 3-5 the velocity field can be obtained as well as other quantities such as pressure distribution and acceleration of individual particles. To determine the position of the free-surface and hence the depths $d_2$ and $d_3$, the average value of the y-coordinate of particles located at the assumed free-surface with half the initial interparticle distance added was used. Particles in the interval of $[1.0 \, 1.1]$ and $[1.5 \, 1.6]$ in the x-direction was used to determine $d_2$ and $d_3$ respectively.

With the present inlet condition $v_1 = 1.5 \, \text{m/s}$ and depth $d_1 = 0.02 \, \text{m}$, $Fr = 3.4$ and consequently $d_2 = 0.086 \, \text{m}$ and $d_3 = 0.058 \, \text{m}$. Results obtained from the simulations of the depths $d_2$ and $d_3$ are summarized in Tables 2-3.

Table 2: The theoretically derived depth $d_2$ and numerical results obtained for the three cases coarse, mid and fine.

<table>
<thead>
<tr>
<th>time [s]</th>
<th>$d_{2, \text{theory}}$ [m]</th>
<th>$d_{2,c}$ [m]</th>
<th>$d_{2,m}$ [m]</th>
<th>$d_{2,f}$ [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.0</td>
<td>0.086</td>
<td>0.083</td>
<td>0.087</td>
<td>0.067</td>
</tr>
<tr>
<td>3.5</td>
<td>0.086</td>
<td>0.082</td>
<td>0.082</td>
<td>0.088</td>
</tr>
<tr>
<td>4.0</td>
<td>0.086</td>
<td>0.083</td>
<td>0.083</td>
<td>0.083</td>
</tr>
<tr>
<td>4.5</td>
<td>0.086</td>
<td>0.084</td>
<td>0.083</td>
<td>0.082</td>
</tr>
<tr>
<td>5.0</td>
<td>0.086</td>
<td>0.081</td>
<td>0.086</td>
<td>0.088</td>
</tr>
</tbody>
</table>

Table 3: The theoretically derived depth $d_3$ and numerical results obtained for the three cases coarse, mid and fine.

<table>
<thead>
<tr>
<th>time [s]</th>
<th>$d_{3, \text{theory}}$ [m]</th>
<th>$d_{3,c}$ [m]</th>
<th>$d_{3,m}$ [m]</th>
<th>$d_{3,f}$ [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.0</td>
<td>0.058</td>
<td>0.060</td>
<td>0.057</td>
<td>0.060</td>
</tr>
<tr>
<td>3.5</td>
<td>0.058</td>
<td>0.056</td>
<td>0.059</td>
<td>0.055</td>
</tr>
<tr>
<td>4.0</td>
<td>0.058</td>
<td>0.058</td>
<td>0.061</td>
<td>0.053</td>
</tr>
<tr>
<td>4.5</td>
<td>0.058</td>
<td>0.058</td>
<td>0.058</td>
<td>0.061</td>
</tr>
<tr>
<td>5.0</td>
<td>0.058</td>
<td>0.058</td>
<td>0.058</td>
<td>0.052</td>
</tr>
</tbody>
</table>

As derived from Tables 2-3 both the coarse and mid cases agrees well with the theoretically derived values of both depths. However, the depths for the fine case oscillates heavily compared to other two. This chaotic behavior might be due to inherent numerical instabilities of the SPH-method satisfying the conclusions of previous works $^{10,11}$. However, it might be the most physically correct solution implying that the threshold of refinement when a divergent behavior is obtained is not reached or it might not be applicable to the current problem. Further validation through experiments is needed in order to confirm which of the above statements is correct. Experiments of current or similar geometrical setup can be found in the literature $^{16}$ hence such analysis has great potential for future work efforts.

As mentioned above, the pressure distribution is easily obtained from simulation data. However, as the pressure was greatly over predicted by the Gruneisen EOS no such figures is
shown. This behavior is at this stage not known to the authors but the validity of the Gruneisen EOS and the parameters used for current problem might be questionable.

5 CONCLUSIONS

The capabilities of the SPH-method to accurately capture the main features of a hydraulic jump such as the transition between supercritical- and subcritical flow has been demonstrated. Furthermore, the dynamics of the highly turbulent roller and the air entrapment process has been visualized even though a single phase has been modeled only. Comparison of theoretically derived values and numerical results of the depth $d_2$ in the subcritical section and the depth $d_3$ in the contraction past the weir show good agreement for the coarse and mid cases. The fine case show oscillating tendencies which might be due to inherent numerical instabilities of the SPH-method or it might show a more physically correct solution. Further validation through experiment is needed to clarify these issues.

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SPH SIMULATION OF SLOSHING DUE TO HORIZONTAL TANK EXCITATION

D.C. SWAPNADIP* AND S.A. SANNASIRAJ†
Department of Ocean Engineering
Indian Institute of Technology Madras (IIT Madras)
Chennai 600036, India
e-mail: dcswapnadip@googlemail.com*, sasraj@iitm.ac.in†, www.oec.iitm.ac.in

Key words: Smoothed particle hydrodynamics (SPH) Simulation, Dam break, Sloshing.

Abstract. Smoothed particle hydrodynamics (SPH), a true mesh less method has been used to simulate the sloshing problem. The tank motion is restricted to regular horizontal excitation. A number of issues have been addressed while making attempts for simulating with higher h/l ratio. The principle approaches undertaken in order to understand the effectiveness of the standard method have been mostly laid upon different boundary modeling techniques and the artificial viscosity models. Selected method for the time integration scheme has been found to play a significant role. The classical dam break problem has been revisited based on those findings. Model predictions for this case have been compared with few other different CFD techniques as well as experimental data as available in literature. Simulation of tank sloshing has been compared with FEM simulation where the entire mode of investigation is different. The fine tuned values of different controlling parameters have been reported.

1 INTRODUCTION

The SPH method was independently developed by Lucy [1] and Monaghan [2] for solving problems in astrophysics. Soon it attracted the research community interested in investigating fluid dynamical problems with its robustness, ease in understanding and inherent non-necessity of following any grid structure. It has been continuously gaining considerable attention from researchers working on particle based methods. Followed by the rigorous works of Monaghan and Kos [3], Dalrymple and Rogers [4] and, Colagrossi and Landrini [5], it has been understood that SPH is an attractive option to simulate water waves when there is a flow separation. Following the successful application of simulating nonlinear free surface waves, SPH has been adopted to simulate sloshing waves. Souto-Iglesias et al. [6] calculated the moment imparted by the inner liquid on the tank wall by using SPH and compared the free surface shape obtained by the same with experimental data. Delorme et al. [7] examined the impact pressure and studied phase lags with respect to the sloshing frequency using both SPH as well as experiments. Both of these last two mentioned studies were performed for the 2D rolling case. Apart from satisfying a number of agreements with experiments which were otherwise would be difficult to observe through conventional methods it triggered certain issues to be investigated further. A number of algorithms were proposed to adopt along with the basic SPH formulation in order to mitigate the deficiencies. The present study examines some of the concepts to successfully simulate sloshing in a container. The tank motion is restricted to regular horizontal excitation.
2 SPH FORMULATION

The foundation of SPH is based on the theory of integral interpolation. It is based on the mathematical representation that any field variable may be decomposed into several differential parts representing the value of the same at that point interpolated from the surrounding set of points. The intensity of an individual interpolation in that process is controlled by a properly chosen kernel function. Therefore in a continuous field, a field variable \( f = f(x) \) may be expressed as

\[
f(x) = \int_{\Omega} f(x') W(x - x', h) dx'
\]  

Whereas, the derivative of \( f(x) \) is written as [8],

\[
f'(x) = \int_{\Omega} f(x') W'(x - x', h) dx'
\]  

The field variable \( f(x) \) at the point \( x \) is obtained from the information of the function at point \( x' \), \( h \) is called the smoothing length which when multiplied by a scale factor \( k \) represents radius of influence around the point \( x \). \( W \) denotes the kernel function which closely approximate the Dirac-delta function as the smoothing length \( (h) \) tends to zero. The choice of the kernel function has been found to be important both in terms of accuracy of the overall interpolation scheme and computational cost. After making few tests on available form of kernel functions, the normalized Gaussian kernel as reported by Colagrossi and Landrini [5] is adopted in the present study based on its better stability properties and efficiency. It is written as,

\[
W(R, \delta) = \frac{e^{-\frac{R^2}{2\delta^2}} - e^{-\frac{\delta^2}{2h^2}}}{2\pi \delta \int_0^{\delta} s \left( e^{-\frac{s^2}{2\delta^2}} - e^{-\frac{s^2}{2h^2}} \right) ds}
\]

where, \( R = s/h \), \( s = r_{ij} \), distance of neighboring particle \( j \) measured from the particle in hand \( i \) and \( \delta = kh \). The computational domain is discretized in terms of particles. Then following the expressions as shown in Eqns. (1) and (2), the continuity and the Euler equation describing a generic flow filed may be written as

\[
\left( \frac{d\rho}{dt} \right)_i = \sum_{j=1}^{N} m_j u_{ij} \nabla_i W_{ij}
\]

\[
\left( \frac{du}{dt} \right)_i = -\sum_{j=1}^{N} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i W_{ij} + g
\]

Here, \( i \) is the particle at which the associated properties have been determined, \( j \) denotes the neighboring particle, \( \rho \) is the density, \( P \) is the pressure, \( m \) is the mass of a particle, and \( g(0, -9.8) \) is the acceleration due to gravity. In both of the above equations, summation is taken over the neighboring particles for a particle for which the calculation
of the desired properties is required. Assuming the fluid medium as weakly compressible, the pressure term appearing in Eqn. (5) is obtained from density as [9],

\[
p = B \left( \frac{\rho}{\rho_0} \right)^\gamma - 1
\]

(6)

The ordinary differential equations thus obtained are integrated with respect to the time for a given interval and the particle positions are updated in subsequent time steps.

3 MODELLING BOUNDARY

There are a number of procedures available for modeling boundaries in SPH. Here, the treatment on rigid boundaries is discussed. Yet, particles are seldom found to go beyond the prescribed domain and thereby collapsing the simulation. The main inconvenience comes from the lack of particles to be taken into account for the interpolation process for a field variable near the rigid boundary. In the present study, three methods for modeling the boundary have been tested as described below.

3.1 Dalrymple dynamic

This method was firstly proposed by Crespo et al [10]. The rigid boundary around the domain is defined by boundary particles set in a staggered way. Then they are made to interact with the fluid particles with the constraint on the governing equations. But those particles are not evolved in time as predicted by the momentum equation. Either they are kept fixed in their original position or moved according to an independently prescribed motion. In this approach, an opposing force is imparted by a boundary particle on an approaching SPH particle following Eqn. (6). For shorter time simulation, this approach has been found to be suitable to model the rigid boundary. However, for longer time simulation where there exist rapid particle movements around the boundary resulting impact loads, the boundary particles could not resist the interior particles to leave the domain.

3.2 Lennard-Jones type repulsion force

In order to assure no leaking of particles in a true sense, Lennard-Jones type repulsion force, an artificial force on the boundary particles has been imposed. This approach has been mostly followed in SPH simulation. In the present study, the Lennard-Jones type force has been used. It is written as

\[
F = \begin{cases} 
D \left[ \left( \frac{r_b}{r_y} \right)^n - \left( \frac{r_b}{r_y} \right)^{n_e} \right] \frac{x_{by}}{r_y^2}, & \text{if } r_y < r_b \\
0, & \text{otherwise}
\end{cases}
\]

(7)
The parameters \( r_o \) which denotes the limit in distance from the boundary over which this force becomes activated and the constants \( D \), \( n_i \) and \( n_2 \) control its effectiveness. The actual values of them have been found to be mostly problem dependent. Too much repulsion would further resulted in the distortion of the flow field.

### 3.3 Ghost particles

Ghost particles (GP) are mirror reflections of SPH particles appearing in the vicinity of a rigid boundary. The approach taken in order to implement this procedure resembles the same adopted by Colagrossi and Labrini [5]. The key idea is to arrange the flow properties of the GPs in such a way that while taking summation for a nearby SPH particle using the GPs as neighbors, it leads to an approximate satisfaction of the free slip condition near the boundary. Most of the initial simulation carried out in our study are using GPs. However, similar to the findings of Delorme et al. [7], there have been some event of particle leaking. So, the above mentioned Lennard-jones type repulsion force has been incorporated with properly calibrated value of the control parameters.

### 4 THE ARTIFICIAL VISCOSITY TERM

The following artificial viscosity term \( \Pi \) appearing in Eqn. (5) is used in the following form [3].

\[
\Pi_{ij} = \begin{cases} 
-\alpha \frac{c_i \mu_{ij} + \beta \mu_{ij}^2}{\rho_{ij}}, & v_{ij} \cdot r_{ij} \leq 0 \\
0, & v_{ij} \cdot r_{ij} > 0 
\end{cases}
\]  

where, \( \mu_{ij} = \frac{h v_{ij} r_{ij}^2}{\rho_{ij}^2 + \eta^2} \), \( r_{ij} = r_i - r_j \), \( v_{ij} = v_i - v_j \), \( c_i = \frac{c_i + c_j}{2} \), \( \rho_{ij} = \frac{\rho_i + \rho_j}{2} \), \( \eta^2 = 0.01 h^2 \), and \( \alpha \) is a parameter which is generally taken in between the range of 0-0.1. In most of the test cases, the value of \( \beta \) is taken as zero. \( C_i \) and \( C_j \) are the numerical sound speeds associated with a particle and calculated according to the particle density at that instant. \( V \) is the velocity vector corresponding to that particle.

### 5 DENSITY REINITIALIZATION

It is well known that the pressure field suffers from huge numerical oscillation in SPH simulation. The main reason behind this is the inablity of the chosen kernel function to retain a certain range of consistency as the model proceeds in time. Therefore the density field which takes a direct control over the pressure field is periodically initialized as [5],
\[
(\rho_{new})_i = \frac{\sum_{j=1}^{N} m_j W_{ij}}{\sum_{j=1}^{N} \rho_j}
\] (9)

The above method referred as Shepard filtering helps to damp out numerical noise in the pressure field. But its effectiveness has been found to be limited in long run. Beyond that it hardly plays any role. So, in the simulation reported herein, the maximum termination time has been fixed up to 10s.

6 TIME INTEGRATION SCHEME

Fourth order Ruge-Kutta (RK4) method along with a dynamic choice of time step has been used to integrate the Eqns. (4) and (5) with respect to time. The time step size (\(dt\)) is made as given by Colagrossi and Landrini [5] in order to satisfy the Courant Friedrichs Levy-type condition as

\[
dt = \theta \min_j \left( \frac{h}{c_{ij} + \sigma_i} \right)
\] (10)

\[
\sigma_i = \max_j \left( h \left| \frac{u_j - u_i}{x_j - x_i} \right| \frac{x_j - x_i}{|x_j - x_i|^2} \right)
\] (11)

The value of \(\theta\) is taken as 2.5 for RK4.

7 RESULTTS AND DISCUSSION

7.1 Dam break

The classical dam break problem has been analyzed to understand the influence of various dictating parameters in SPH simulation. The problem is shown schematically in Fig. 1. Here a dam is represented by a vertical column of water retained by a gate initially. Then the gate is released instantaneously. The test case has been carried out for a domain length (L) of 1m. Fig. 2 shows snap shots for particle configurations taken at different instant of time. Table 1 presents the different input parameters adopted in the dam break simulation.
Table 1: Dam break: input data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum expected flow velocity (Vmax)</td>
<td>$2\sqrt{gh}$</td>
</tr>
<tr>
<td>$\alpha, \beta$ as in Eqn. (8)</td>
<td>1.8, 2.03</td>
</tr>
<tr>
<td>D as in Eqn. (7)</td>
<td>$0.5 V_{max}^2$</td>
</tr>
<tr>
<td>$n_1, n_2$ as in Eqn. (7)</td>
<td>12, 6</td>
</tr>
<tr>
<td>$r_i$ in Eqn. (7)</td>
<td>0.25$\Delta x$</td>
</tr>
<tr>
<td>Smoothing length (h)</td>
<td>0.66$\Delta x$</td>
</tr>
</tbody>
</table>

Figure 1: The problem geometry for the dam break problem
Figure 2: Snap shots showing particle configurations taken at every 0.25 s intervals for the dam break problem

Fig. 3 shows the plot of normalized position of the water front measured along the horizontal axis against normalized time ($t_s = t\sqrt{2g/l}$). It also shows a comparison with MPS [12] and VOF [14] simulation results as well as experimental measurements [13]. The comparison of present SPH simulation with the experimental measurements is found to be good.
7.2 Tank sloshing  The sloshing in a rectangular tank subjected to regular horizontal excitation has been simulated. The problem domain is shown in Fig. 4 along with the coordinate system. The tank excitation, $X(t)$ is prescribed by

$$X(t) = a_x \cos(\omega t) \quad (12)$$

![Figure 4: Sloshing tank](image)

Figure 3: Comparison for the dam beak case with other methods and experiment.
Here, $a_n$ is the amplitude of oscillation and $\omega_n$ is the excitation frequency. The different input parameters used to follow a particular test case so as to compare with FEM simulation [11] are given in Table 2.

<table>
<thead>
<tr>
<th>Table 2: Input parameters for the sloshing problem</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length of the tank (L)</td>
</tr>
<tr>
<td>Still water depth (h)</td>
</tr>
<tr>
<td>Amplitude of oscillation ($a_n$)</td>
</tr>
<tr>
<td>Excitation frequency ($\omega_n$)</td>
</tr>
</tbody>
</table>

Here, $\omega_1$ is the first mode of natural frequency written for the generic modes as

$$\omega_n = \sqrt{gk_n \tanh (k_nh)} \quad n = 1, 2, 3.. \quad (13)$$

$k_n = n\pi / L$, is the wave number.

Table 3 presents the different input parameters adopted during SPH simulation. Here $dx$ refers to the initial particle spacing.

<table>
<thead>
<tr>
<th>Table 3: Tank sloshing: input data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum expected flow velocity ($V_{\text{max}}$)</td>
</tr>
<tr>
<td>$\alpha$, $\beta$ as in Eqn. (8)</td>
</tr>
<tr>
<td>D as in Eqn. (7)</td>
</tr>
<tr>
<td>$n_1$, $n_2$ as in Eqn. (7)</td>
</tr>
<tr>
<td>$r_o$ in Eqn. (7)</td>
</tr>
<tr>
<td>Smoothing length (h)</td>
</tr>
</tbody>
</table>

Fig. 5 shows snap shots of particle configuration taken at every 1.5 s intervals starting from the initial configuration for the above problem.
Figure 5: Particle snapshots taken after every 1.5s intervals starting from the initial configuration.

Now, the time history of the free surface elevation at the top left corner of the tank is compared with Sriram et al. [11] which was based on fully nonlinear potential flow theory in Fig. 6.
The SPH simulation of free surface time history at the left wall of the tank shows good comparison with the fully nonlinear potential flow theory simulation up to 3s. Beyond that the particles have been found to get scattered to such an extent that affects the local interpolation process for calculating the field variables of a particle. Then the solution sought after the model has been found to diverge from the actual values. In overall, it can be seen that the energy level decreases continuously over the period of simulation. Numerical damping is the main factor behind such variation. Due to the artificial increase of the damping, there is a phase shift. Even though, numerical damping is believed to be a common problem for any numerical method which solves the Navier-Stokes equation, SPH has shortcomings by introducing such numerical damping through various factors such as smoothing length and artificial viscosity. Yet, it motivates the authors to investigate further over these issues.

8 CONCLUSIONS

In recent times it has been well known that the difficulties associated with grid based methods to capture a wave breaking or rapidly changing free surface are dealt through mesh less methods like SPH. But it suffers from lack of accuracy prior to non-breaking as when compared with well established methods. This paper checks SPH in its standard form and reports its output in long time simulations. The present study focuses on the simulation of sloshing in a rectangular tank forced by regular wave excitation using SPH. The various factors that affect the simulation process have been tested. A proper control
of input parameters has been found to improve the accuracy. However, a number of unresolved issues have been observed which require further investigations.

9 REFERENCES

A 3D GENERALIZED RIGID PARTICLE CONTACT MODEL FOR ROCK FRACTURE

N. MONTEIRO AZEVEDO*, J. LEMOS*

* Concrete Dams Department
Laboratório Nacional de Engenharia Civil (LNEC)
Av. Do Brasil 101, 1700-066 Lisboa Portugal
e-mail: {nazevedo, vlemos} @lnec.pt, www.lnec.pt/organizacao/dbb

Key words: DEM, Contact model, Fracture, Rock.

Abstract. Detailed rigid particle models have been proposed for modeling fracture in quasi-brittle materials. The rigid particle circular models proposed in the literature do not properly reproduce the known rock friction angle and the observed rock tensile strength to compression strength ratio. In this article, a 3D rigid particle contact model, 3D-GCM, is presented which has been developed to study fracture phenomena in rock. The 3D-GCM contact model incorporates in a straightforward manner the force versus displacement relationships of the traditional contact point contact model, PCM. Furthermore it provides both moment transmission and simple physical constitutive models based on standard force displacement relationships. The 3D-GCM model is validated against known triaxial and Brazilian tests of a granite rock. It is shown that the enhanced rigid particle model leads to a better agreement with the experimental results.

1 INTRODUCTION

Detailed rigid particle models have been introduced in the study of fracture of continuous media such as concrete and rock in the early 1990's [1-6]. More recently 3D rigid spherical particle models have been proposed for rock, [7, 8], and for concrete, [9-11]. Models based on the rigid spring block method adopting 3D Voronoi shape polyhedra have also been developed for concrete, [12-13].

Through the simulation of the material meso-structure, the rigid particle models prevent localization of damage into regions not sufficiently large when compared to the inhomogeneity size. Particle models are conceptually simpler than a continuum approach, and the development of cracks and rupture surfaces appears naturally as part of the simulation process given its discrete nature. As discussed in Cundall [14], assemblies of discrete particles connected through simple interaction laws are able to capture the global behaviour of quasi-brittle macro-material, like concrete or rock. The parameters of the interaction laws may require some calibration at the micro-level.

In rock fracture studies the bonded particle model, BPM, [8] has received considerable attention given its known ability to model rock complex behaviour, namely in uniaxial compression. It adopts the traditional single point contact model, PCM, for grain behaviour, in parallel with a contact model that allows moment transmission through a rotational
stiffness spring, parallel bond, PB, which attempts to simulate the cement behaviour. The BPM model, as presented in [8], is not able to model the ratio of tensile strength to compressive strength that occurs in rock. Also the macroscopic friction angle obtained through triaxial testing is quite low when compared to the known rock experimental values.

In this work, a 3D generalized contact model, 3D-GCM, based on the 2D contact model [15] is presented. The number of local points used in the contact discretization is a model parameter and can be set to a given value. With the 3D-GCM it is still possible to model the traditional PCM contact model adopting only one contact point. By increasing the density of local contact points the elastic response converges to the response obtained with the PB contact model which adopts a uniform distribution of local points [8]. The proposed model is validated against known triaxial and Brazilian tests in a granite rock. It is shown that the enhanced rigid particle model leads to a better agreement with the known experimental results.

2 FORMULATION

2.1 Fundamentals

In the DEM, the domain is replaced by an assembly of discrete entities that interact with each other through contact points or contact interfaces. The ability to include finite displacements and rotations, including complete detachment, and to recognize new contacts as the calculation progresses are essential features. The set of forces acting on each particle are related to the relative displacements of the particle with respect to its neighbours. At each step, given the applied forces, Newton's 2nd law of motion is invoked to obtain the new position of the particle. The equations of motion, including local non-viscous damping, of a particle may be expressed as:

\[
F_i(t) + F^d_i(t) = m \ddot{x}_i + m \dot{x}_i \\
M_i(t) + M^d_i(t) = I \omega_i + I \dot{\omega}_i
\]  \hspace{1cm} (1)

where: \( F_i(t) \) and \( M_i(t) \) are, respectively, the total applied force and moment at time \( t \) including the exterior contact contribution, \( m \) and \( I \) are, respectively, the particle mass and moment of inertia, \( \ddot{x}_i \) and \( \dot{x}_i \) are the particle acceleration and velocity, \( \omega_i \) and \( \dot{\omega}_i \) are, respectively, the particle angular acceleration and velocity. The damping forces are given by:

\[
F^d_i(t) = -\alpha |F_i(t)| \text{sign}(\dot{x}_i) \\
M^d_i(t) = -\alpha |M_i(t)| \text{sign}(\dot{\omega}_i)
\]  \hspace{1cm} (2)

being, \( \dot{x}_i \) the particle velocity and \( \alpha \) the local non-viscous damping and the function \text{sign} (x) given by:

\[
\text{sign}(x) = \begin{cases} 
+1, & x > 0 \\
-1, & x < 0 \\
0, & x = 0
\end{cases}
\]  \hspace{1cm} (3)
2.2 Generalized contact model (3D-GCM)

The 3D-GCM as defined is based on the 2D-GCM contact model that considers on a given contact width a discrete number of local contact points that are able to transfer normal and shear forces [15]. In the 3D-GCM contact model, one can have on an idealized cylindrical contact surface, several concentric circular clouds of contact points, Figure 1.

![Diagram of 3D-GCM contact model discretizations](image)

**Figure 1**: 3D-GCM contact model discretizations

The number of layers and the total number of points per layer is a model parameter. As the number of contacts points is increased, one obviously obtains the equivalent continuum solution, PB contact model [8]. Given the contact surface discretization, it is possible to
transfer through the contact surface both force, bending and torsional moments. As referred, the traditional PCM contact model only allows the transmission of force. The contact unit normal is defined given the particles centre of gravity and the inter-particle distance, see Figure 1a):

\[ n_j = \frac{x_j^{[g]} - x_j^{[A]}}{d} \]  

\hfill (4)

The contact overlap for the reference contact point and its location are given by:

\[ U^n = R^{[A]} + R^{[B]} - d \]
\[ x_i^{[0]} = x_i^{[A]} + \left( R^{[A]} - \frac{1}{2} U^n \right) n_i \]  

\hfill (5)

In the 3D-GCM contact model it is further required to set for each local contact point, its contact location and local contact overlap. For this reason, a local \((t,s)\) axys is defined, Figure 1b). Given the contact discretization one needs to know for each local contact point, its local coordinates relative to the reference contact point. Then the local contact point position in global coordinates can be defined using:

\[ x_i^{[j]} = x_i^{[0]} + s^{[j]} x_j^{[s]} + t^{[j]} x_j^{[t]} \]  

\hfill (6)

where: \(x_j^{[s]}\) and \(x_j^{[t]}\) are the global coordinates of the local \(s\) axys and local \(t\) axys, respectively. The contact forces that are acting on each local contact point can be decomposed into its normal and shear component with respect to the contact plane:

\[ F_i^{[s]} = F_i^{[s,t]} + F_i^{[t,s]} \]  

\hfill (7)

The contact velocity of a given local contact point, which is the velocity of particle \(B\) relative to particle \(A\), at the contact location is given by:

\[ \dot{x}_i^{[j]} = \dot{x}_i^{[B]} - \dot{x}_i^{[A]} = \left( \dot{x}_i^{[B]} + \epsilon_{ik} \omega_k^{[B]} (x_i^{[j]} - x_i^{[b]}) \right) - \left( \dot{x}_i^{[A]} + \epsilon_{ik} \omega_k^{[A]} (x_i^{[j]} - x_i^{[a]}) \right) \]  

\hfill (8)

The contact displacement normal increment, \(\Delta x_i^{[j,N]}\), stored as a scalar, and shear increment, \(\Delta x_i^{[j,S]}\), stored as a vector, are given by:

\[ \Delta x_i^{[j,N]} = (\dot{x}_i^{[j]} \Delta t) n_i \]
\[ \Delta x_i^{[j,S]} = (\dot{x}_i^{[j]} \Delta t) - \Delta x_i^{[j,N]} n_i \]  

\hfill (9)

The local contact point overlap is defined incrementally for all the local points based on the current contact velocity time step, \(\Delta t\):
Given the normal and shear stiffness of the local contact point, the normal and shear forces increments are obtained following an incremental linear law:

\[ \Delta F_{J,n} = -k_n \Delta x_{J,n} \]
\[ \Delta F_{J,s} = -k_s \Delta x_{J,s} \]

The predicted normal and shear forces acting at the local contact point are then updated by applying the following equations:

\[ F_{J,n,\text{new}} = F_{J,n,\text{old}} + \Delta F_{J,n} \]
\[ F_{J,s,\text{new}} = F_{J,s,\text{old}} - \varepsilon_{ijk} \varepsilon_{kmn} F_{J,s,\text{old}} n_m n_n + \Delta F_{J,s} \]

Due to the fact that the shear contact force is stored in global coordinates, it is necessary to redefine it in the updated contact plane. Given the predictive normal and shear contact forces, the adopted constitutive model is applied. If the predictive forces do not satisfy the constitutive model an adjustment, that is model dependent, needs to be carried. The resultant contact force at the local contact point is then given by:

\[ F^J = F_{J,n} n_i + F_{J,s} \]

At the reference contact point, the resultant contact force and contact moment are defined given the contribution from all the contact points:

\[ F_{i}^{[c]} = \sum F_{i}^{J} \]
\[ M_{i}^{[c]} = -\sum \varepsilon_{ijk} (x_{j}^{0} - x_{j}^{i}) F_{k}^{J} \]

The contact force and moment are then transferred to the particle centre of gravity of each particle in contact through:

\[ F_{i}^{[A]} = F_{i}^{[A]} - F_{i}^{[c]} \]
\[ F_{i}^{[B]} = F_{i}^{[B]} + F_{i}^{[c]} \]
\[ M_{i}^{[A]} = M_{i}^{[A]} - \varepsilon_{ijk} (x_{j}^{0} - x_{j}^{i}) F_{k}^{[c]} - M_{i}^{[c]} \]
\[ M_{i}^{[B]} = M_{i}^{[B]} + \varepsilon_{ijk} (x_{j}^{0} - x_{j}^{i}) F_{k}^{[c]} + M_{i}^{[c]} \]
2.3 Numerical stability

When only a steady state solution is sought, a mass scaling algorithm is adopted in order to reduce the number of time steps necessary to reach the desired solution. The particle mass and inertia are artificially scaled so the centred-difference algorithm has a higher rate of convergence for a given loading step. The particle scaled mass and inertia, used in the calculations are set assuming a unit time increment, given the particle stiffness at a given time through:

\[ m_{\text{scaled}} = 0.25 \, k_j \quad I_{\text{scaled}} = 0.25 \, k_\rho \]  

(17)

The total translation stiffness \( k_t \) and the rotational stiffness \( k_\theta \) of each particle must include the contribution of all particles in contact at a given time step:

\[
\begin{align*}
    k_t &= \sum_{i=1}^{N_c} \left( \sum_j k_n^j + \sum_j k_s^j \right) \\
    k_\theta &= \sum_{i=1}^{N_c} \left( K_s d_{AC}^2 + K_s d_{BC}^2 + 2K_s R^2 + 2K_n R^2 \right)
\end{align*}
\]

(18)

where:

\[
K_s = \sum_j k_s^j, \quad K_s R^2 = \sum_j k_s^j \left( (s_j^i)^2 + (t_j^i)^2 \right)
\]

and

\[
K_n = \sum_j k_n^j \left( (s_j^i)^2 + (t_j^i)^2 \right)
\]

2.4 Local contact stiffness and local contact strength

In this work the total 3D-GCM contact stiffness associated to the contact is given by:

\[
\begin{align*}
    K_n &= \frac{E}{d} \frac{\pi R^2}{d} \\
    K_s &= \eta K_n
\end{align*}
\]

(19)

where: \( \overline{R} \) is minimum radius of the particles in contact, \( d \) is the distance between the particles in contact, \( E \) is the Young modulus of the equivalent continuum material and \( \eta \) is a constant that relates the normal and the shear stiffness spring value. The total tensile and shear contact strength are defined given the maximum stresses and the contact area by:

\[
\begin{align*}
    F_{\text{t,n}} &= \overline{\sigma_n} \pi \overline{R}^2 \\
    F_s &= \pi \tau \overline{R}^2
\end{align*}
\]

(2)

The contact properties, strength and stiffness of each local contact point are then defined given the contact local weight and the total contact values. In this work the same weight is given to the local points. For the local inter-particle contacts, a brittle Mohr-Coulomb model including a frictional term before failure with tension cut-off is adopted, Figure 2. As soon as
the maximum shear or tensile strength is reached the local contact is considered to be cracked only transferring forces under compression.

![Figure 2: 3D-GCM local contact constitutive model](image)

2.5 Particle generation scheme

The particle assemblies here presented have been generated using the algorithms proposed in [8]. The initial circular particle assembly is created by first inserting the particles with half their radius guaranteeing that the particles do not overlap with each other, Figure 3a). Then the particle real radius is adopted, and a DEM cohesionless type solution is obtained, leading to a redistribution of the particle overlap throughout the assembly. The final assembly, Figure 3b), is obtained by setting the desired initial isotropic stress, followed by a floater elimination procedure, [8].

![Figure 3: Particle assembly for a granite rock](image)

The particle assemblies generated, similar to the presented in [8], are then triangulated using a Delaunay scheme. In this work it is considered that two particles interact with a GCM contact model if they share a common Delaunay tetrahedron edge, even if they are not in real contact. When compared to the particle assemblies presented in [8], where only particles closer than $1 \times 10^{-6}$ of the average radius are considered to be in contact, the number of connections is significantly increased.
3 TRIAXIAL AND BRAZILIAN TEST IN A GRANITE ROCK

The 3D-GCM model is validated against triaxial and Brazilian tests in a granite rock (Lac du Bonet) [8]. The tests were performed in cylindrical specimens with a 0.0634 m height and 0.0317 m radius. Two different particles assembly sizes were adopted. A coarser assembly with a uniform diameter distribution ranging from 1.50 mm to 2.49 mm, with a total average of 7800 particles. And a finer particle assembly, with a uniform diameter distribution ranging from 1.19 mm to 1.98 mm, with 15600 particles in average.

In the triaxial tests the initial isotropic pressure is applied through the vertical and lateral confinement walls, Figure 4a). After setting the isotropic stress, a small downward velocity is given to the upper vertical wall, \(0.25 \times 10^{-8}\) m/s, in order to simulate quasi-static conditions. The lateral walls are subdivided into several polyhedral pieces that do not interact with each other and can only have inward displacement, in order to approximate the behaviour of a flexible membrane. Also with this purpose, the lateral wall contacts with the spherical particles have a lower stiffness, around 10% of the inter-particle stiffness. In the Brazilian tests the quasi-static load is applied by giving a downward velocity, \(0.75 \times 10^{-9}\) m/s, to the upper plate.

![Figure 4: Particle assemblies – Boundary conditions](image)

Table 1 presents the micromechanical elastic and strength properties that were adopted for the different particle assemblies adopted. Given some difficulties in matching the Poisson ratio of the Lac du Bonet granite (\(\nu = 0.26\)) it was also assessed a GCM model with different spring stiffness for tensile and compression loading. For the GCM contact a local discretization of 5 local points was adopted, one central point and four peripherical local points, all with the same local weight. The strength micro-parameters were calibrated on a trial and error basis in order to match the experimental uniaxial compression strength and the Brazilian test tensile strength.
Table 1: Micro-properties for Lac du Bonet granite

<table>
<thead>
<tr>
<th></th>
<th>$K_n$ (tension)</th>
<th>$K_n$ (compression)</th>
<th>$\sigma_{n,t}$ [MPa]</th>
<th>$\tau$ [MPa]</th>
<th>$\mu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCM-A1</td>
<td>50.0</td>
<td>-</td>
<td>0.25</td>
<td>33.5</td>
<td>43.5</td>
</tr>
<tr>
<td>GCM-A2</td>
<td>24.0</td>
<td>48.0</td>
<td>0.30</td>
<td>25.0</td>
<td>33.0</td>
</tr>
<tr>
<td>GCM-B1</td>
<td>50.0</td>
<td>-</td>
<td>0.25</td>
<td>33.0</td>
<td>44.0</td>
</tr>
<tr>
<td>GCM-B1</td>
<td>24.0</td>
<td>48.0</td>
<td>0.30</td>
<td>25.0</td>
<td>33.5</td>
</tr>
</tbody>
</table>

Table 2 presents the macro strength properties obtained with the different particles assemblies and contact models. It can be identified that a spring with reduced value under tensile loading increases the Poisson ratio. In order to match the Poisson ratio with a constant spring stiffness it would be necessary to adopt a constant $\eta = \frac{K_n}{K_i}$ lower than 0.07, which can be considered to be quite low. In [8] a similar mechanism was adopted, the cemented contacts, PB type, work under compression in parallel with granular type contacts, and under tensile loading only the PB contacts carry the tensile loading. The macroscopic friction angle and the cohesion values are set according to the expressions defined in [8] that take as input the triaxial results. Lac du Bonet granite is considered to have an average friction angle of 59º and a cohesion value of 30 MPa [8]. The numerical macroscopic friction angle is still lower than the Lac du Bonet value, $\phi = 59.0^\circ$, but it is in much better agreement when compared with the numerical value obtained in [8] ($\phi = 32.1^\circ$) with an equivalent spherical model and particle assembly. The uniaxial maximum compression values are also in good agreement with the Lac du Bonet granite that has a known average value of 200.0 MPa.

Table 2: Macro-properties for Lac du Bonet granite

<table>
<thead>
<tr>
<th></th>
<th>$E$ [GPa]</th>
<th>$\nu$</th>
<th>$q_u$ [MPa]</th>
<th>$\phi$ [º]</th>
<th>$C$ [MPa]</th>
<th>$\sigma_t$ [MPa]</th>
<th>$q_u/\sigma_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCM-A1</td>
<td>72.8</td>
<td>0.19</td>
<td>202.1</td>
<td>44</td>
<td>42.5</td>
<td>28.7</td>
<td>7.0</td>
</tr>
<tr>
<td>GCM-A2</td>
<td>72.7</td>
<td>0.24</td>
<td>201.6</td>
<td>40</td>
<td>47.5</td>
<td>28.5</td>
<td>7.1</td>
</tr>
<tr>
<td>GCM-B1</td>
<td>74.0</td>
<td>0.18</td>
<td>205.5</td>
<td>46</td>
<td>41.6</td>
<td>26.4</td>
<td>7.8</td>
</tr>
<tr>
<td>GCM-B1</td>
<td>73.5</td>
<td>0.23</td>
<td>203.3</td>
<td>43</td>
<td>43.9</td>
<td>24.3</td>
<td>8.4</td>
</tr>
</tbody>
</table>

Table 2 also shows that the 3D-GCM contact model with a brittle contact law is not able to model the ratio of compression strength to tensile strength. The Lac du Bonet granite has a known 21.5 ratio. This shows that the 3D-GCM contact model needs to be further enhanced, for example by considering the fracture energy at the micro-level.
Figure 5: Strength envelope for the 3D-GCM models and experimental testing [8]

Figure 5 compares the strength envelope results obtained with the 3D-GCM contact model with an equivalent spherical particle model [8] and with the experimental results obtained for Lac du Bonet granite [8]. It can be seen that the 3D-GCM contact model leads to a better agreement with the known Lac du Bonet strength envelope.
Figure 5a) presents the strength envelope obtained with a zero micro-mechanical
friction angle, $\mu = 0.0$, GCM-A3. Note that the latter strength envelope is close to the obtained with an equivalent spherical model that also does not include the friction angle at the inter-particle contact [8]. This shows that the friction angle value, that can be straightforwardly included within a GCM-contact formulation, is relevant in order to have a better agreement with the known experimental value.

12 CONCLUSIONS

A generalized 3D contact model, 3D-GCM, is presented which is defined through identifiable mechanisms of shear and normal force transfer through the contact interface. In this paper, the GCM contact model is adopted in the interaction between particles that share a common tetrahedron edge. Note that when compared to other particle models for rock [8] each particle has a higher number of particle interactions.

The 3D-GCM contact model incorporates in a straightforward manner the force versus displacement relationships of the traditional contact point contact model model, PCM, providing both moment transmission and simple physical constitutive models based on standard force displacement relationships. The results indicate that 4 local points at the outer boundary of the contact are sufficient in order to obtain complex macro-responses.

It is also shown that 3D-GCM model between spherical particles by incorporating a frictional term at the inter-particle contact level leads to a more realistic hard rock macroscopic behaviour, namely the macroscopic friction angle is increased.

Finally, the 3D-GCM contact model with a brittle contact law is not able to model the ratio of compression strength to tensile strength of the Lac du Bonet granite. It is expectable to have a better agreement with the real response if a more complex contact constitutive law, e.g. softening at the contact level, is incorporated within a 3D-GCM contact model.

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A TANGENTIAL FORCE-DISPLACEMENT MODEL FOR ELASTIC FRICTIONAL CONTACT BETWEEN PARTICLES IN TRIAXIAL TEST SIMULATIONS

PIETER FRANKEN*, STIJN FRANÇOIS*, ENGELBERT TIJSKENS† AND GEERT DEGRANDE*

*Department of Civil Engineering, K.U.Leuven
Kasteelpark Arenberg 40, B-3001 Leuven, Belgium
web page: http://bwk.kuleuven.be/bwm
e-mail: Pieter.Franken@bwk.kuleuven.be

†Department of Biosystems, K.U.Leuven
Kasteelpark Arenberg 30, B-3001 Leuven, Belgium

Key words: Discrete Element Method, Triaxial Test, Tangential Contact Model, Granular Soil

Abstract. A tangential contact model for three-dimensional discrete element simulations is proposed and used in the micro-mechanical simulation of a drained triaxial test. In this model, the dependence of the tangential contact force on the contact loading history is accounted for. A representative volume element with spherical discrete elements and periodic boundary conditions is used in the simulations to reduce the computation costs. Numerical results of a triaxial test obtained with a linear and the proposed tangential contact model are compared. The results for both contact models are qualitatively in agreement with theory. The linear contact model needs calibration as the used parameters lack physical meaning, while the proposed contact model only uses physical properties of the particles.

1 INTRODUCTION

A phenomenological approach, where parameters are used to describe the behaviour observed in physical tests, such as triaxial tests, is frequently used to study the behaviour of granular soils. When studying accumulation phenomena in granular soils resulting from repeated small amplitude dynamic loading, however, phenomenological models exhibit limitations. Current accumulation models [7, 13] use a large number of parameters that often lack physical meaning. As a result, little insight in the physical processes is gained, while an extensive amount of laboratory tests has to be performed for model calibration.
As an alternative, a micro-mechanical approach can be followed, which has the potential to overcome the limitations of current phenomenological models. The discrete element (DE) method [3] is commonly applied for the study of granular materials under monotonic, static loads [12]. In this method, the equations of motion are solved for each particle, depending on the interaction with other particles. The contact law has a large influence on the constitutive behaviour of the sample. Since many microscopic properties are difficult to measure or model, simplifications are often made to the contact law. Linear models are mainly used for calculating the contact forces [1, 5]. Contact models based on the contact theories for elastic frictional contact, such as the theory of Hertz [9] for the normal component and Mindlin and Deresiewicz [11] for the tangential component, yield more realistic results. Hertz’ contact theory is frequently used to compute the normal contact force [4, 6].

As the tangential contact force depends on the loading history of a contact, a linear incremental relation between the tangential displacement and the contact force is mostly applied. In order to incorporate the loading history, Walton and Braun [20] proposed a tangential contact model which is a simplification of the Mindlin-Deresiewicz contact theory, where several different loading histories are considered. Walton and Braun only distinguished between an increasing or decreasing tangential force. Vu-Quoc and Zhang [18] improved the model of Walton and Braun by considering 4 loading cases of the Mindlin-Deresiewicz theory for a varying normal contact force. The model of Walton and Braun is still applied when the normal force is constant.

A more realistic tangential contact model for elastic frictional contact is proposed [8], consisting of 16 loading cases which are based on 7 loading cases of the Mindlin-Deresiewicz contact theory. According to the contact theory, the model only makes use of scalar quantities. The three-dimensional (3D) implementation utilizes the framework by Vu-Quoc et al. [19]. Subsequently, numerical results of a triaxial test with the proposed contact model and a linear visco-elastic tangential contact model are compared.

The present study is a first step towards the development of a realistic micro-mechanical model of granular soils under repeated cyclic loading.

2 THE TANGENTIAL CONTACT MODEL

Hertz [9] studied the normal contact between elastic spheres. Starting from this theory, Mindlin and Deresiewicz [11] developed a contact theory for varying normal and tangential components of the contact forces. As the tangential component depends on the loading history, the theory is divided in a variety of loading cases. Based on the contact theory, an incremental solution is proposed, which is only valid when the increments in the normal $\Delta F_n$ and the tangential $\Delta F_t$ contact forces are small. In each loading case, the tangential contact force increment is given by:

$$\Delta F_t = K_t \Delta u_{rel}^{el}$$ (1)
where $K_t$ is the tangential stiffness at the current time step, which incorporates the loading history, and $u_t^{rel}$ is the tangential component of the relative displacement between two contacting particles. The superscript ‘rel’ is omitted in the following as all displacements and velocities in this paper refer to the relative values between two particles in contact. The theory of Mindlin and Deresiewicz [11] is developed considering the stress distribution over the contact area between spherical particles. The distribution of the normal stress $\sigma_n(\rho)$ over a circular contact area is given by Hertz’ theory [9]:

$$\sigma_n(\rho) = \frac{3F_n}{2\pi a^3} \sqrt{a^2 - \rho^2}$$  \hspace{1cm} (2)

where $a$ is the radius of the contact surface and $\rho$ varies between 0 and $a$. This stress distribution results from the normal contact force $F_n$, which is related as follows to the relative normal displacement $u_n$ of the two spheres:

$$F_n = \frac{4\sqrt{R_{\text{eff}}E_{\text{eff}}}}{3} u_n^{3/2}$$  \hspace{1cm} (3)

where $1/R_{\text{eff}} = (R_1 + R_2)/(R_1R_2)$ is the relative contact curvature and $E_{\text{eff}}$ is the effective elastic modulus, defined as:

$$E_{\text{eff}} = \left(\frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2}\right)^{-1}$$  \hspace{1cm} (4)

where $\nu_1$ and $\nu_2$ are the Poisson’s ratios and $E_1$ and $E_2$ the Young’s moduli of the two spheres in contact.

The distribution of the tangential stress $\tau$, and thus the tangential contact force $F_t$, cannot be written in closed form as it depends on the loading history. Considering the case where the normal force is constant, the tangential force as a function of the relative tangential displacement $u_t$ is given by a hysteresis curve shown in figure 1. The tangential stiffnesses, which relate the tangential force with the relative tangential displacement, are given by [11]:

$$K_t = K_{t0} \left(1 - \frac{F_t}{\mu F_n}\right)^{1/3} \text{ for } \dot{F}_t > 0 \text{ and } |F_t| \geq F_{t,\text{max}}^{\text{tp}} \text{ (curve 1)}$$  \hspace{1cm} (5)

$$K_t = K_{t0} \left(1 - \frac{F_{t,\text{max}}^{\text{tp}} - F_t}{2\mu F_n}\right)^{1/3} \text{ for } \dot{F}_t < 0 \text{ and } |F_t| < F_{t,\text{max}}^{\text{tp}} \text{ (curve 2)}$$  \hspace{1cm} (6)

$$K_t = K_{t0} \left(1 + \frac{F_{t,\text{max}}^{\text{tp}} - F_t}{2\mu F_n}\right)^{1/3} \text{ for } \dot{F}_t > 0 \text{ and } |F_t| < F_{t,\text{max}}^{\text{tp}} \text{ (curve 3)}$$  \hspace{1cm} (7)

$$K_t = K_{t0} \left(1 + \frac{F_t}{\mu F_n}\right)^{1/3} \text{ for } \dot{F}_t < 0 \text{ and } |F_t| \geq F_{t,\text{max}}^{\text{tp}} \text{ (curve 4)}$$  \hspace{1cm} (8)

Equations (5) to (8) show that the tangential stiffness depends on the normal contact force $F_n$, the tangential contact force $F_t$, the tangential contact force at the last turning
point $F_{t}^{tp}$, the maximal tangential force at a turning point $F_{t,max}^{tp}$, the coefficient of friction $\mu$ and the initial tangential stiffness $K_{t0}$:

$$K_{t0} = 8a \left( \frac{2 - \nu_1}{G_1} + \frac{2 - \nu_2}{G_2} \right)^{-1}$$  \hspace{1cm} (9)

where $G_1$ and $G_2$ are the shear moduli of the two contacting spheres. The maximal tangential force $F_{t,max}^{tp}$ is defined as the highest absolute value of the tangential force at a turning point occurred in the history of the contact.

![Figure 1: Tangential force $F_t$ as a function of the tangential component $u_t$ of the relative displacement for constant normal loading.](image1)

![Figure 2: Tangential force $F_t$ as a function of the relative tangential displacement $u_t$ for increasing normal and tangential force, while $|F_t^{i-1}| \geq F_{t,max}^{tp}$.](image2)

The case with a constant normal contact force occurs only in special configurations. The normal and tangential components of the contact force mostly vary arbitrarily. To account for this in DE calculations, equations (5) to (8) are approximated numerically, resulting into 16 loading cases [8] which depend on the loading history. The loading cases are divided in four main groups: (1) increasing normal force, increasing tangential force; (2) increasing normal force, decreasing tangential force; (3) decreasing normal force, increasing tangential force and (4) decreasing normal force, decreasing tangential force. These groups are based on the four loading cases defined by Vu-Quoc and Zhang [18], where the condition of an increasing/decreasing force is evaluated at the current time step.

In contradiction to the model of Vu-Quoc and Zhang, a distinction is made between the tangential force at the last turning point $F_{t}^{tp}$ and the maximal tangential force $F_{t,max}^{tp}$. In many cases, these parameters are equal, e.g. point A for curve 2 (figure 1). If point C is the last turning point (e.g. $F_{t}^{tp} = F_{t,C}$ on curve 5), the values of these parameters differ and a distinction is needed between $F_{t}^{tp}$ and $F_{t,max}^{tp}$ as the tangential stiffness depends on both. Four different loading situations can therefore be defined within each of the groups, cf. equations (5) to (8). These loading cases are defined based on the variation and value
of the tangential force at the previous time step \( i - 1 \): (1) \( F_{t}^{i-1} \) increasing, \(|F_{t}^{i-1}| \geq F_{t,\text{max}}^{\text{tp}}\); (2) \( F_{t}^{i-1} \) decreasing, \(|F_{t}^{i-1}| < F_{t,\text{max}}^{\text{tp}}\); (3) \( F_{t}^{i-1} \) increasing, \(|F_{t}^{i-1}| < F_{t,\text{max}}^{\text{tp}}\) and (4) \( F_{t}^{i-1} \) decreasing, \(|F_{t}^{i-1}| \geq F_{t,\text{max}}^{\text{tp}}\).

The solution of Mindlin and Deresiewicz \cite{11} is limited to simple loading histories, which are defined as a sequence of equilibrium positions. An equilibrium position is a state which can be achieved by holding the normal force constant at the current value and varying the tangential force. Every point on the curve of figure 1 corresponds to an equilibrium position for one specific value of the normal contact force.

In the following, as an example, the loading case of the first group (increasing normal force, increasing tangential force), where \( F_{t}^{i-1} \) is increasing and \(|F_{t}^{i-1}| \geq F_{t,\text{max}}^{\text{tp}}\), is discussed. An analogous procedure is used for the other 15 loading cases \cite{8}.

**The loading case for \( F_{n}^{i}, F_{t}^{i} \) and \( F_{t}^{i-1} \) increasing and \(|F_{t}^{i-1}| \geq F_{t,\text{max}}^{\text{tp}}\)**

According to the Mindlin-Deresiewicz theory \cite{11}, the increment in the tangential contact force is achieved by first changing the normal force while the tangential force remains constant and then changing the tangential force under constant normal force. This means that first the normal force is increased to \( F_{n}^{i} = F_{n}^{i-1} + \Delta F_{n} \). The values of \( F_{t}^{\text{tp}} \) and \( F_{t,\text{max}}^{\text{tp}} \) are set to zero since this case corresponds to curve 1 in figure 1, where no turning point has yet occurred (figure 2). Then, under constant normal force, the tangential force is increased through a sequence of equilibrium positions (‘simple loading history’) until the final state is reached (figure 2, from state 0 to state 2). Two subcases are derived: \( \Delta F_{t} \geq \mu \Delta F_{n} \) and \( \Delta F_{t} < \mu \Delta F_{n} \). Since \( \Delta F_{t} \) is unknown, these subcases are changed into \cite{21} \( \Delta u_{t} \geq (\Delta u_{t})_{01} \) and \( \Delta u_{t} < (\Delta u_{t})_{01} \), where the displacement from state 0 to state 1 \( (\Delta u_{t})_{01} = \mu F_{n}^{i} / (K_{t})_{01} \). The tangential stiffness \((K_{t})_{01}\) is taken constant and equal to the initial stiffness \( K_{t0} \) for a loading under constant normal force \( F_{n}^{i} \). The latter is only true when the increment in the normal force \( \Delta F_{n} \) is small.

When \( \Delta u_{t} \geq \mu \Delta F_{n} / K_{t0} \), as indicated in figure 2, the subsequent tangential force is given by:

\[
F_{t}^{i} = (F_{t})_{1} + (K_{t})_{12} (\Delta u_{t})_{12} = F_{t}^{i-1} + \mu \Delta F_{n} + (K_{t})_{12} \left( \Delta u_{t} - \frac{\mu \Delta F_{n}}{K_{t0}} \right) \tag{10}
\]

where the tangential stiffness \((K_{t})_{12}\) is equal to (cf. equation (5)):

\[
(K_{t})_{12} = K_{t0} \left( 1 - \frac{F_{t}^{i-1} + \mu \Delta F_{n}}{\mu F_{n}^{i}} \right)^{1/3} \tag{11}
\]

When \( \Delta u_{t} < \mu \Delta F_{n} / K_{t0} \), the subsequent tangential force is given by:

\[
F_{t}^{i} = F_{t}^{i-1} + K_{t0} \Delta u_{t} \tag{12}
\]

However, the final state in equation (12) does not correspond to an equilibrium position, as it is not equivalent to a state of constant normal force and varying tangential force. The loading is therefore no longer part of a simple loading history. This causes inaccuracies, since the model is based on the assumption of simple loading histories.
3 IMPLEMENTATION IN 3D DISCRETE ELEMENT METHOD

To use the proposed tangential contact model in a 3D DE method requires vector manipulation since the model is only valid for a 2D model where the tangential plane at a contact point reduces to a line.

First, it is assumed that the orientation of the contact plane remains constant. In a 3D simulation, the direction of the tangential force in the tangential plane varies during the simulation. As a result, the above scalar model is not applicable. Nevertheless, the model can be applied in a 3D simulation if the components $F_t^\parallel$ and $F_t^\perp$ of the tangential force parallel and perpendicular to the initial relative tangential displacement increment $\Delta u_{t0}$ are considered [19]. The model is then applied in each direction separately. The direction of $F_t^\parallel$ is equal to $t^\parallel = -\Delta u_{t0}/||\Delta u_{t0}||$. The minus sign shows that the tangential force on a particle is opposite to the relative displacement of that particle.

After the directions of the tangential force components have been determined, the model proposed in the previous section can be applied. An increase or decrease in the tangential force $F_t$ is derived from the sign of the relative tangential displacement increment $\Delta u_t$, since the increment in each component $\Delta F_t^\parallel$ and $\Delta F_t^\perp$ of the tangential force is always opposite to the corresponding component $\Delta u_t^\parallel$ and $\Delta u_t^\perp$ of the relative tangential displacement increment (figure 3). For example, when $\Delta u_t^\parallel$ is opposite to $t^\parallel$, the components $u_t^\parallel$ and $F_t^\parallel$ of the relative tangential displacement and the tangential force parallel to the initial tangential displacement are increasing. The increment $\Delta F_n = F_n^i - F_n^{i-1}$ in the normal force and the tangential force $F_t^{i-1}$ at the previous time step determine which loading case applies to the current time step. In the implementation of the model, the loading cases with a constant normal force are not considered, because the cases where the normal force is increasing converge towards the cases with a constant normal force.

![Figure 3: Positive increments of the relative tangential displacement and the tangential force shown in the tangential contact plane.](image)

After application of the tangential model, the two components of the tangential force at the current time step $i$ are known. These components, however, may not exceed the Coulomb friction limit, which determines the value of the tangential force in case of sliding: $|F_t^\parallel| \leq \mu F_n^i$ and $|F_t^\perp| \leq \mu F_n^i$. 

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So far, the directions and the values of the two components of the tangential force are calculated assuming the orientation of the tangential plane remains constant through the simulation. To account for the change in orientation of the contact plane, the direction of the components is corrected in each time step. The direction at the previous time step is projected onto the tangential contact plane at the current time step:

$$t_i^\parallel = t_i^{\parallel - 1} - (t_i^{\parallel - 1} \cdot n^i) n^i$$  \hspace{2cm} (13)

$$t_i^\perp = t_i^{\perp - 1} - (t_i^{\perp - 1} \cdot n^i) n^i - (t_i^{\perp - 1} \cdot t_i^\parallel) t_i^\parallel$$  \hspace{2cm} (14)

where $n^i$ is the unit normal vector of the tangential contact plane at time step $i$. This is less accurate than a rotation around the contact point, but acceptable since the force and displacement increments are small. The latter is a requirement of the tangential force-displacement model and inherent to the DE method. The third term in equation (14) ensures that $t^\perp$ is always perpendicular to $t^\parallel$.

Finally, the total tangential force in time step $i$ is given by:

$$F_i^t = F_i^{t\parallel} + F_i^{t\perp} = F_i^{t\parallel} t_i^\parallel + F_i^{t\perp} t_i^\perp$$  \hspace{2cm} (15)

Since this force has a larger value than each of its components, the Coulomb friction limit $|F_i^t| \leq \mu F_n^i$ is additionally enforced.

4 TRIAXIAL TEST SIMULATIONS

The proposed contact model is applied in the micro-mechanical simulation of a drained triaxial test and implemented in the DE software program $DEMeter++$ [17].

The results are compared to results of a triaxial test simulation with a linear visco-elastic tangential contact model. The linear contact model is also applied incrementally:

$$F_i^t = \min \left( F_i^{t - 1} - K_{\text{lin}} \Delta u_i - A_{\text{lin}} K_{\text{lin}} \Delta v_i, \mu F_n \frac{F_{t_i}^{\text{el}}}{||F_i^t||} \right)$$  \hspace{2cm} (16)

where $F_i^{t - 1}$ is the elastic part of the tangential force at the previous time step $i - 1$, $K_{\text{lin}}$ is a constant tangential stiffness, $A_{\text{lin}}$ is a dissipative coefficient and $v_i$ is the relative velocity between two contacting spheres.

The normal contact force, in both simulations, is given by Hertz’ theory (equation (3)), extended with a term to account for the dissipation of energy in every contact [14]:

$$F_n = \frac{4E_{\text{eff}} \sqrt{R_{\text{eff}}}}{3} \left( u_n^{3/2} + A_n \sqrt{u_n} \nu_n \right)$$  \hspace{2cm} (17)

where the dissipative coefficient is taken equal to $A_n = 10^{-8}$ to ensure the stability of the calculations without affecting the results. This term is only added during the isotropic compression of the sample (section 4.1).

A soil sample with a diameter of 5 cm, a height of 12 cm and a mean particle diameter of 1 mm is used in the simulations. For a dense sand with a porosity $n = 0.35$, a huge
amount of particles are needed to simulate a full-scale triaxial test, which results in very high computation costs. Therefore, only a part of the soil sample is considered, indicated in figure 4a as a representative volume element (RVE). This RVE is much smaller than the soil sample, but large enough to give meaningful results.

Figure 4: (a) Representative volume element (RVE) and (b) soil sample under triaxial conditions.

The simulation of a triaxial test is performed using a cubic RVE which contains 817 spherical particles. The micro-mechanical properties of the particles are based on the properties of quartz sand [16]: $E = 70$ GPa, $\nu = 0.3$, density $\rho_s = 2650$ kg/m$^3$ and friction coefficient $\mu = 0.3$. The parameters $K_{lin}$ and $A_{lin}$ for the linear contact model are found by calibrating the linear model to the proposed contact model. A poorly graded sand is used where the radii of the spheres follow a log-normal distribution with an average of 0.5 mm and a standard deviation of 0.05 mm. The minimum and maximum values for the radii are equal to 0.35 mm and 0.71 mm, respectively.

The RVE is modeled with periodic boundaries to represent the behaviour of the whole sample and avoid boundary effects. To control the deformation of the RVE the particles are subjected to a strain-rate tensor $\dot{\epsilon}_{ij}$ in addition to the displacements resulting from the interaction with other particles. A servo-control algorithm relates the strain-rate tensor to the stress tensor, which enables to follow stress-controlled loading paths [16]:

$$
\left( \frac{\Delta \epsilon_{ij}}{\Delta t} \right)^i = \left( \frac{\Delta \epsilon_{ij}}{\Delta t} \right)^{i-1} + g (\sigma^d_{ij} - \sigma^{i-1}_{ij})
$$

where $\sigma^d_{ij}$ is the target stress tensor, $\sigma^{i-1}_{ij}$ is the calculated stress tensor at the previous time step and $g$ is a gain parameter which value is obtained by trial and error [16]. A good value for $g$ is found when the target stress path is followed correctly. The stress tensor is obtained as a volume average over all the contacts:

$$
\sigma_{ij} = \frac{1}{V} \sum_{c=1}^{N_c} l_{ci} F_{cj}
$$

where $V$ is the volume of the RVE, $N_c$ is the total amount of contacts, $l_{ci}$ is the $i$-th component of the contact vector for contact $c$ connecting two particles at their centers and $F_{cj}$ is the $j$-th component of the contact force vector at that contact. Equation (18)
may be expressed in terms of individual or combinations of components of the strain-rate and stress tensors, depending on the loading path followed [16]. Since a triaxial test is a special case where the principal stresses $\sigma_i$ are known (figure 4b), only these stresses are controlled by equation (18) and the corresponding strain rates $\dot{\epsilon}_i$ are applied to the particles to control the deformation of the RVE.

Due to the high Young's modulus, the critical time step is very small. The estimation of the critical time step [10] is based on an infinite series of point masses $m$ connected with springs $k$. The smallest period, and thus the critical time step, occurs when the masses are moving in counter-phase, such that there is no motion at the center of each spring. A very small time step of $\Delta t = 10^{-7}$ s is then obtained.

To allow for a larger time step, density-scaling is applied [16]: the density is scaled up by a factor $b = 10^{12}$, as the forces $F$ and displacements $dx$, which determine the stresses and strains, are not affected by the scaling. The accelerations $a$ and velocities $v$ are reduced by factors $b$ and $\sqrt{b}$, respectively, but these quantities are not important when considering quasi-static behaviour. The following values for the density and time step are thus applied: $\rho_s = 2650 \times 10^{12}$ kg/m$^3$ and $\Delta t = 0.1$ s.

4.1 Sample preparation

The RVE is created by random placement of the spherical particles, without overlapping, in a cubic volume with initial side length of 10 mm. The porosity is initially equal to $n = 0.55$. The sample is isotropically compressed to a mean normal stress $p = -100$ kPa, using principal strain rates, calculated with equation (18), with an initial value of $\dot{\epsilon}_1 = \dot{\epsilon}_2 = \dot{\epsilon}_3 = -10^{-4}$/s, a maximal value of $|\dot{\epsilon}|_{\text{max}} = 10^{-4}$/s and a gain parameter of $g = 10^{-7}$. In order to create a dense assembly, the friction coefficient is set to zero during the isotropic compression [16]. Prior to the triaxial test simulation, the friction coefficient is adjusted to $\mu = 0.3$. When applying the proposed tangential contact model, the porosity and mechanical average coordination number (amount of contacts per particle) after isotropic compression are $n = 0.3517$ and $Z_m = 4.68$, respectively. When applying the linear contact model, the porosity and mechanical average coordination number after isotropic compression are $n = 0.3518$ and $Z_m = 4.71$, respectively. This shows that the initial conditions for the two simulations are almost equal.

4.2 Triaxial test

A static triaxial test is performed by increasing the axial pressure $\sigma_1$ under constant confining stress $\sigma_2 = \sigma_3 = \sigma_c = -100$ kPa. The increase in the axial pressure is carried out in a strain controlled manner: a constant strain rate of $\dot{\epsilon}_1 = -10^{-5}$/s is applied vertically to the top and bottom of the RVE. The stresses $\sigma_2$ and $\sigma_3$ are held constant by applying the servo-control algorithm (equation (18)) with an initial value for the strain rates of $\dot{\epsilon}_2 = \dot{\epsilon}_3 = 0$ and a gain parameter of $g = 10^{-9}$.
The stress-strain behaviour for the simulation with the proposed tangential contact model is shown in figure 5 (black curve). A qualitative agreement with the theory of critical state soil mechanics [2, 15] is observed: yielding starts at a strain value of about 3%, after which a strain-softening and dilative behaviour is observed, converging to a constant deviatoric stress and volumetric strain. The critical state line is reached at about 30% axial strain.

![Figure 5: Stress-strain behaviour of the triaxial test simulation with the proposed tangential contact model (black) and a calibrated linear tangential contact model (gray): (a) deviatoric stress and (b) volumetric strain as a function of the axial strain.](image)

Calibration of the two simulations yields values of $K_{\text{lin}} = 10^5 \text{ N/m}$ and $A_{\text{lin}} = 1$ for the parameters of the linear contact model. With these values, the results of the two simulations are almost equal (figure 5). This illustrates that the stress-strain behaviour in a triaxial test is mainly governed by the normal contact model, which is the same in both simulations. The benefit of the proposed tangential contact model is that, while the parameters in the linear contact model have no physical meaning, it only makes use of physical properties of the particles, which are also used in the normal contact model (equation (17)): the Poisson’s ratio $\nu$, the Young’s modulus $E$ and the friction coefficient $\mu$. The proposed model does not need calibration when the microscopic properties of the soil are known. The friction coefficient, however, is difficult to determine as it is function of the surface roughness of the particles. Nevertheless, the use of physical properties is expected to result in a more profound understanding of the behaviour of granular soils as insight is gained in the physical processes at micro-scale.

5 CONCLUSIONS

A tangential force-displacement model is proposed for elastic frictional contact between spherical particles, which is based on the theory by Mindlin and Deresiewicz [11]. The contact loading history is accounted for by considering 16 different loading cases. This results in an accurate evaluation of the tangential contact force. Since the model only makes use of scalar quantities, a 3D implementation of the model is given which requires vector
manipulation to keep track of the orientation of the tangential force and the evaluation of this force has to be done for each of its components separately.

A drained triaxial test on a dense sand is simulated, which is qualitatively in correspondence with the theory of critical state soil mechanics [2, 15]. The comparison of numerical results of a triaxial test obtained with the proposed and a linear tangential contact model shows the minor influence of the tangential contact force to the stress-strain behaviour compared to the normal contact force. The parameters of the proposed contact model have a physical meaning, which is expected to result in a more profound understanding of the micro-mechanical behaviour of granular soils.

REFERENCES


ADVANCED MONITORING AND NUMERICAL TECHNIQUES FOR ASSESSING THE STABILITY OF TUNNELS

HAN-MEI CHEN*, PROF HAI-SUI YU† AND DR MARTIN SMITH‡

*Nottingham Centre for Geomechanics, Faculty of Engineering, The University of Nottingham
Email: evxhc@nottingham.ac.uk
† Email: hai-sui.yu@nottingham.ac.uk
‡ Institute of Engineering Surveying and Space Geodesy, Faculty of Engineering, The University of Nottingham
Email: martin.smith@nottingham.ac.uk

Key words: Advanced Monitoring techniques, Tunnel Stability.

Abstract. This research aims to develop an advanced monitoring technique for assessing the stability of tunnels, which may substitute or supplement the conventionally manual procedures.

In this paper, ‘laser scanning technique’ is primarily studied to determine the utilisation of laser scanners for condition monitoring of lined tunnels. A series of model tests have been
carried out by using laser scanning technology, in which models were set up simulating tunnel conditions. After scanning and processing in the corresponding software, 3D coordinates of the models were obtained as well as 3D ‘point clouds’ models. Thus various defect targets like cracks and deformation on the tunnel wall could be identified and measured efficiently in these digital models. Precision and limitations related to laser scanning were also highlighted. In addition, numerical simulation would also be conducted using FLAC$^{2D}$ and FLAC$^{3D}$ software to link the simulated tunnel behaviours to overall structural stability.

This study indicates that laser scanning technique has potential for executing condition monitoring, such as depth and width of cracks, deformation of tunnels, with high accuracy in a static mode of scanning. By these observed information combined with numerical analysis, the stability of the tunnels could be assessed for safety.

1 INTRODUCTION

Most tunnels in UK are built decades ago, some are even over a hundred years old. Degradation and tunnel deformation are major threats to tunnel’s stability which lead to a collapse of a tunnel if not controlled. Therefore monitoring and examination of tunnels are important to diagnose the deterioration and conduct repair work, before serious damage occurs.

Tunnel inspection has predominantly been a manual procedure, which is time-consuming and subjective, giving rise
to variance in standards and quality of examinations for tunnels. The overall aim of the study is to develop an automated technique which may substitute or augment the manual tunnel examination survey in the demand for higher efficiency as well as standardisation of tunnel inspections. Initially, a series of laboratory tests are conducted to study the utilisation of laser scanning system for condition monitoring of lined tunnels.

Furthermore, numerical models are needed to be developed according to the current monitoring results, to predict and assess the future status of the tunnel.

2 LABORATORY WORK WITH THE TERRESTRIAL LASER SCANNING (TLS) SYSTEM

2.1 Brief introduction to the TLS system

The TLS technique has been recognised as a promising tool in the field of engineering over the past few years as it quickly provides a realistic representation of objects [1]. Moreover, the TLS system provides dense point clouds of the scanned surface coordinates to build a 3D model of the target. As several papers revealed the potential of laser scanning in accurately mapping surface displacements in underground excavations [1] and detecting damage parts on tunnel walls [5], it would be very interesting to utilise the TLS for condition monitoring in tunnels, such as crack depth and the deformation of tunnels.

There are two laser scanners employed in the experimental work, namely a RIEGL LMS-Z420i laser scanner and an
improved laser scanner, the RIGEL VZ-400. It is expected that the scanning results for the later would be collected faster and have a better performance in respect of accuracy.

2.2 Designed test models

Intact model 1: The bricks used in the first model are brand-new red, smooth Norman bricks. Each brick is $215 \times 105 \times 73$mm (L×W×H). The bond pattern is ‘Stretcher bond’ inserting a half-brick setting every second row. Figure 1 shows that the whole model has been divided into 9 test areas each with different brickwork properties.

![Figure 1: The division of model 1](image)
The aim of setting up this model was to establish what the scanner could detect in undamaged brickwork and to form a base model reference for different systems.

**Figure 2:** The division of model 2 (Surface texture & cracks)

Model 2 (with cracks & surface texture): The second model (Figure 2) has been separated into 2 parts. The bricks of upper part are a mixture of smooth, pattern textured, and reclaimed bricks. The reclaimed bricks simulate weathered bricks in railway tunnels to see how brick texture could influence the scanner. The lower part of the model uses smooth bricks as in model 1. It contains roughly 11 narrow artificial cracks throughout the area, each of which is approximately 3mm wide.
It also contains a big crack 12mm wide and a small void. The brick spacing in model 2 is 10mm. The entire model was built without mortar to simulate heavily recessed weathered mortar in real railway tunnels and to establish how far the scanner could see into the open joints.

The objective of setting up this model was to discover the influence of the texture of the brick surface as well as to determine the visibility of the laser scanner on deep narrow cracks and deep mortar depth.

2.3 Laboratory and measuring work

The experimental work was carried out by both laser scanners separately at the measuring distance from 2m, 4m to 6m (Figure 3). After that, all the measurements were conducted manually in the software by taking an average, such as measuring mortar depth, crack width and brick spacing width.
2.4 Post-processing results and discussions

After initial data processing and measuring work with the RiSCAN PRO software, the results to be discussed are listed:
1) Comparison of images for different angular resolutions using the LiDAR RIGEL VZ-400
2) Comparison of the LiDAR RIGEL VZ-400 & LMS-Z420i on results for
   • Accuracy of mortar depth
   • Noise from the brick surface (after triangulation)
   • Possibility of measuring width of brick spacing and cracks

The factors influencing the accuracy of laser measurement such as weathered mortar depth are concluded here:
• Physical accuracy and beam divergences of different laser scanner
• Hand-made measuring accuracy on the software
• Inclined scan direction effect: (Illustrated in Figure 4)
• Skew scan direction effect: (Illustrated in Figure 5)
• Different measuring distances: For instance, with the RIGEL VZ-400, an angular resolution of 0.041° could achieve a discrepancy of 2% for the average measurement of mortar depth up to a distance of 6m. While at the distance of 2m, the discrepancy is around 9%.
• Different angular resolutions: In theory, the smaller the angular resolution is, the better the accuracy is. Whereas it is not practical to use the very small resolution with much
more scan time. Therefore various angular resolutions are set up to find an appropriate one with high accuracy.

![Figure 4: The potential indentation between bricks by laser beam](image)

![Figure 5: The plan view of scanning process](image)

3 NUMERICAL MODELLING OF ROCK TUNNELS

3.1 Modelling of an unlined rock tunnel

Model assumptions: The total model size chosen for a series of model tests is 207m wide by 87m deep (See Figure 6). For model simplification, only half of the model (103.5m wide by 87m deep) is simulated in FLAC$^{2D}$ considering the model section symmetry. A horseshoe tunnel is 30m below the surface, 100m away from either left or right boundary of the model, sized 7m wide, 3.5m for both side walls and radius 3.5m for the arch. Both left and right boundaries are fixed in x-direction, and the bottom boundary is fixed in y-direction.
Figure 6: Geometry of the model with boundary conditions

The tunnel is only subjected to the self weight of the surrounding rock which is homogeneous. The density of the rock is 2700 kg/m³. The top boundary of the model domain represents a free surface.

Different values of rock mechanical parameters as cohesion (C), friction angle (φ), elastic modulus (E) and Poisson’s ratio (ν) were chosen for each modelling test shown in Table 1, to find the influence of rock material on tunnel stabilization.

Table 1: Basic values of mechanical parameters for each test

<table>
<thead>
<tr>
<th>Friction angle (°)</th>
<th>Poisson's ratio</th>
<th>Elastic modulus (GPa)</th>
<th>Cohesion (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35</td>
<td>0.3</td>
<td>50</td>
<td>0.8</td>
</tr>
<tr>
<td>20</td>
<td>0.2</td>
<td>0.5</td>
<td>0.5/0.2/0.15</td>
</tr>
</tbody>
</table>
Modelling results and discussion

Deformation status: Two hyperbolic curves in Figure 7 similarly demonstrate that relatively lower cohesion of the rock around tunnel (e.g. 60KPa) would induce a larger displacement at tunnel invert. From the cohesion above 500KPa, the invert displacement is stable to 0.173mm. In the two graphs, the elastic modulus changes from 50GPa to 0.5GPa. Accordingly, the displacement of the invert centre point at the same cohesion is increased. The displacement shows a linear relation with elastic modulus.

![Figure 7: Relation between cohesion of the rock and the displacement of the tunnel invert](image)

Yield status: In general, the yield area enlarges gradually as the cohesion decreases. Cohesion is the most effective parameter corresponding to the tunnel failure compared with other parameters, by studying the contour outputs.
4 CONCLUSIONS AND FUTURE WORK

4.1 Laboratory work

The presented studies showed the great potential of laser scanning in tunnel monitoring work. In future laboratory work, some improvements would be studied using laser scanners, such as to overcome the angle effect and to have a series of moving scanning processes to increase the scanning speed through a tunnel section.

4.2 Data post-processing

The measuring work for brick spacing and mortar depth has done manually using the RiSCAN PRO software which is not accurate enough. Further automated analysis techniques such as Matlab are needed to be developed for better precision.

4.3 Numerical modelling

Both concrete lining and steel arches have been modelled basically to study the mechanical behaviour of the weak rock tunnel. The next step will specially focus on simulating brickwork arches as a form of railway tunnel support, which will be much challenging due to the composite complexity.

Using FLAC$^{2D}$ could not simulate tunnels surrounded by un-uniform geotechnical materials. Therefore, more work need to be done using FLAC$^{3D}$ as a 3D mode.
5 REFERENCES


ANALYSIS OF MICRO-PROPERTIES FOR TRIAXIAL BEHAVIOUR ON COARSE AGGREGATES USING DEM

MAURICIO A. TAPIAS *, EDUARDO E. ALONSO * AND JOSEP A. GILI *

* Department of Geotechnical Engineering (ETSECCPB)
Universidad Politècnica de Cataluña
Edificio D2, Campus Norte UPC
Gran Capitán s/n, 08034 Barcelona, Spain
e-mail: mauricio.tapias@upc.edu

Key words: Granular Materials, DEM.

Abstract. This paper presents an analysis of the mechanical behaviour of coarse granular aggregates using the discrete element method. A background reference for the conducted study is the set of results of a few large scale triaxial tests performed at the UPC geotechnical laboratory. The basic tool used to simulate some of the tests is the computer code PFC3D. Rockfill particles (they have the size of gravels, typically ranging from 1 cm to 4 cm) were simulated as breakable clusters of 3D balls. Particle breakage occurs in time according to fracture mechanic’s laws. The relationship between stress intensity at a given particle, the size of an initial defect (crack) and the relative humidity could be established. This information was introduced in the numerical analysis to derive criteria for particle breakage in time. The paper describes the preliminary results of the work in progress. The influence of some properties such as particle shape, porosity, toughness, and friction coefficient was studied. The actual shape of rock gravels has been approximated by means of clusters of spherical particles. Several arrangements, comprising a different number of particles, have been tested, having always as reference validation criterion the results from triaxial tests performed. The results of the modelling exercise are encouraging and test results are reasonably well reproduced. The model is fairly general and it has a number of interesting capabilities.

1 INTRODUCTION

Coarse aggregates studied here have gravel size, typically ranging from 1 cm to 4 cm. Two different grain size distributions were studied: uniform and well-graded. In the tests performed Relative Humidity (RH) was controlled by means of a vapour equilibrium technique. The RH existing on the large pores between rock fragments controls the velocity of crack propagation within the particles. An increase in RH means a faster crack propagation and eventually the breakage of some particles and the subsequent re-arrangement of the granular structure. The results of these tests are the background reference for this study.

The paper presents the results of few numerical simulations of triaxial tests using a discrete particle method though the computer code PFC3D.

The final objective of this work is to develop a ‘virtual’ laboratory tool for rockfill


2 A MODEL FOR COARSE GRANULAR AGGREGATES

A series of testing programs on gravels, performed under Relative Humidity control have stressed the relevance of particle breakage in observed macroscopic scale (Chávez & Alonso, 2003; Oldecop & Alonso, 2001; Oldecop & Alonso, 2004; Ortega, 2010). Particle breakage is controlled by the stress level, the current RH and the time.

DEM methods are potentially useful to analyze these effects. The facility to reprogram the code PFC3D through the language FISH and the ‘clump’ logic (creation of group of particles to model particle shapes) has been extensively used. In the results reported the clumps are also known as ‘macroparticles’ to distinguish them from the basic spherical particles (microparticles).

Actual particle shapes tested were formed by 4, 5, 13, and 14 microparticles (Fig. 1). The triaxial tests simulated reproduce the dimensions used in the triaxial experiments performed at UPC (Fig. 2):

- Sample size: Φ:25cm; h:50cm.
- Size of macroparticles: 3 cm. The results reported here correspond to uniform initial grain size.

Tables 1 and 2 provide some fundamental properties for the simulation.

An important practical aspect is to ensure that particles do not carry any contact force before applying the real confining stress. Clumps are generated in a random manner and a desired porosity is imposed. A relaxation of internal forces is then necessary before testing.

**Table 1. Rockfill properties.**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus, E (MPa)</td>
<td>400</td>
</tr>
<tr>
<td>Poisson’s ratio, n</td>
<td>0.4</td>
</tr>
<tr>
<td>Density (Kg/m³)</td>
<td>2760</td>
</tr>
</tbody>
</table>

**Table 2. Properties of macroparticles in DEM model.**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal stiffness, Kn</td>
<td>2e7 N/m</td>
</tr>
<tr>
<td>Shear stiffness, Ks</td>
<td>2e7 N/m</td>
</tr>
<tr>
<td>Friction coefficient, μ</td>
<td>0.93 – 0.5 – 0.3</td>
</tr>
</tbody>
</table>

**Fig. 1.** Rockfill macroparticle. Real and clump models of 1, 4, 5, 13 and 14 microparticles.
3 FAILURE CRITERIA OF PARTICLES

The following issues are discussed regarding the adopted procedure to simulate particle breakage:
• Stress calculations on macroparticles
• Failure criteria for macroparticles
• Division of macroparticles

3.1 Stress in macroparticles

The concept of stress is defined for a representative elementary volume –REV- (ITASCA, 2008; Bagi, 1996, 1999). The REV in our case is the macroparticle. The following procedure was implemented in the code: a) Identify the clump; b) Identify contacts with neighbouring clumps; c) Identify forces in contacts; d) Calculate the mass centroid of the clump; e) Calculate the average stress tensor through the expression (Alonso_Marroquin & Herrman, 2005):

\[
\bar{\sigma}_y = \frac{1}{V} \sum_{a\beta} l_{\alpha}^{a\beta} f_j^{a\beta}
\]  

where \( l_{\alpha}^{a\beta} \): Position vector between mass centroid and contact point; \( \alpha \): Particle; \( \beta \): Contact; \( V \): Volume of macroparticle

Principal stresses are derived from the stress invariants for each macroparticle.
3.2 Failure criteria for macroparticles

Two failure criteria were compared: a classical Mohr Coulomb criterion and a criterion based on the propagation of cracks inside particles (Oldecop & Alonso, 2007). The second criterion is based on linear elastic fracture mechanics (LEFM).

The Mohr-Coulomb criterion requires two parameters for macroparticles: cohesion, $c$, and internal friction coefficient, $\mu$.

The crack propagation criterion is particularly useful because it allows the consideration of suction and time effects. The classical result for a mode of failure (say Mode I for failure in tension, $\sigma$) specifies that whenever the stress intensity factor $K$ reaches the toughness of the rock ($K_c$) a fissure will propagate catastrophically and the rock particle will break. $K$ is defined in terms of a characteristic size $a$:

$$K = \beta \sigma \sqrt{a}$$

where $\beta$ is a dimensionless coefficient which depends on particle geometry.

However, a subcritical propagation of fractures, when $K<K_c$, is also possible (Atkinson, 1984; Oldecop & Alonso 2001). Oldecop and Alonso (2007) describe a phenomenological model, based on subcritical crack growth, for the time to reach particle breakage. The model includes the effects of suction and time.

The approach followed here is to assign a random distribution of defects (cracks) to the macroparticles. Crack length follows a given statistical distribution. The factor $K$, which increases as the crack propagates, is calculated for the minor principal stress which corresponds to a tension state. $K$ for each macroparticle increases also with the applied external stress to the sample tested.

For every time instant of calculation, $K$ is compared with $K_c$. Whenever $K \geq K_c$ the particle is broken in two parts. This is the phenomenon included in all the simulations reported here.

3.3 Particle division

The particle division follows an arbitrary criterion which takes into account the number of particles integrating a clump and the ‘pyramidal’ structure of the macroparticle. Clumps are divided following the ‘rule’: $13 \rightarrow 9+4; 9 \rightarrow 5+4; 5 \rightarrow 3+2; 4 \rightarrow 2+2; 3 \rightarrow 2+1; 2 \rightarrow 1+1$.

Figure 3 provides a comparison of the two criteria (Mohr Coulomb and LEFM) together with a case of no particle breakage. The simulated triaxial test exhibits the highest strength when no particles break, followed by the Mohr Coulomb rupture criterion.

4 SIMULATED TRIAXIAL TESTS

4.1 Particle Shape

Clump sizes of 1; 4(3+1); 5(4+1); 13(9+4); 14(9+4+1), which try always to simulate a pyramidal shape, were tested. Some results are given in Figure 4. The highest peak strengths are found for the highest number of particles in a clump.
4.2 Porosity

The effect of two porosities (51% and 61%) on triaxial test results is given in Figure 5. In both cases the initial macroparticle system had no initial contact forces. The sample exhibiting the lower porosity resulted in the higher stiffness, a consistent result with experimental observations. However, similar peak strength was calculated for the two specimens, a result which is probably explained by particle breakage.
4.3 Contact Stiffness

Three samples having particle to particle normal stiffnesses $k_n$ equal to $2 \times 10^6$, $2 \times 10^7$, and $2 \times 10^8$ N/m respectively were tested in a triaxial experiment. All particles have friction coefficient ($\mu$) equal to 0.3 ($\phi = 17^\circ$). Initial porosity was 51%, the initial confining stress 1 MPa and the toughness of macroparticles was $1 \times 10^4$ Pa√m. The specimen was defined by 970 macroparticles and the initial equivalent diameter was 2.8cm.

Figure 6 shows the deviatoric stress-strain relationship. Samples with greater contact stiffnesses in the micro level (particle to particle) have greater stiffnesses at the macro level, and they get higher peak strengths.

Dilatancy is shown in Figure 7. As expected, dilatancy increases with contact stiffness. This effect is reflected also on the change in porosity during testing (Fig. 8).

The sample having the smallest $k_n$ exhibited a higher number of failed clumps. This sample had the lowest number of not broken clumps (Fig. 9). This is reflected on the calculated grain size distribution at the end of the test (Fig. 10). Crushing in these samples result in an increase in particles having a equivalent diameter close to 2cm and 2.6cm.
4.3 Toughness

Particle toughness is a key property in the fracture model selected. Four values were compared: 1e6 Pa√m; 1e5 Pa√m; 1e4 Pa√m and 1e2 Pa√m. In all cases a triaxial sample having an initial porosity of 0.51 and a confining stress of 1 MPa was tested. Some results are given in Figures 11, 12 and 13.

Toughness controls the peak strength (Fig. 11) although ‘residual’ values seem to be less affected. Samples having a higher $K_c$ value exhibit also a stronger dilatancy (Fig. 12). The lower the $K_c$ value the higher the number of particles ruptured during the test. This is reflected on the calculated grain size distribution at the end of the test (Fig. 13). Crushing in
these samples result in an increase in particles having a equivalent diameter close to 2cm. It is clear that much more deformation energy will be required to achieve an stationary grain size distribution.

These are reasonable results which help to increase the confidence on the model.

Fig. 11. Effect of macroparticle toughness on deviatoric behaviour. Comparison among four different macro-toughness (1e6, 1e5, 1e4, 1e2 Pa\(\sqrt{m}\)). Sample of 1000 macroparticles using clumps of 14 microparticles. Confining stress: 1.0MPa. Initial porosity: 51%.

Fig. 12. Effect of macroparticle toughness on volumetric behaviour. Comparison among four different macro-toughness (1e6, 1e5, 1e4, 1e2 Pa\(\sqrt{m}\)). Sample of 1000 macroparticles using clumps of 14 microparticles. Confining stress: 1.0MPa. Initial porosity: 51%.

Fig. 13. Effect of macroparticle toughness on the evolution of grain size distribution. Comparison among four different macro-toughness (1e6, 1e5, 1e4, 1e2 Pa\(\sqrt{m}\)). Sample of 1000 macroparticles using clumps of 14 microparticles. Confining stress: 1.0MPa. Initial porosity: 51%.

4.4 Friction Coefficient

Three samples having particle to particle friction coefficient (\(\mu\)) equal to 0.93, 0.50 and 0.30 (\(\phi = 43^\circ; 27^\circ; 17^\circ\)) were tested in a triaxial experiment. Initial porosity was 51%, the
initial confining stress 1 MPa and the toughness of macroparticles was $1 \times 10^4$ Pa√m. The specimen was defined by 970 macroparticles and the initial equivalent diameter was 2.8 cm.

Figure 14 shows the deviatoric stress-strain relationship. A similar residual strength for strains in excess of 20% was found. Dilatancy is shown in Figure 15. As expected, dilatancy increases with interparticle friction. In this test most of the particles broken resulted in equivalent particle diameters in the vicinity of 2 cm. The sample having the smallest interparticle friction angle exhibited a higher number of failed clumps.

Only a small percentage of particles broke in these tests. More will be said on this aspect in the next section.

![Fig. 14. Friction coefficient effect on deviatoric behaviour. Comparison among three friction coefficients (0.93, 0.50, 0.30). Sample of 1000 macroparticles using clumps of 14 microparticles. Confining stress: 1.0 MPa. Initial porosity: 51%.](image1)

![Fig. 15. Friction coefficient effect on volumetric behaviour. Comparison among three friction coefficients (0.93, 0.50, 0.30). Sample of 1000 macroparticles using clumps of 14 microparticles. Confining stress: 1.0 MPa. Initial porosity: 51%.](image2)

5 RELATIVE HUMIDITY EFFECTS

Investigating the effect of Relative Humidity on rockfill behaviour is one of the main objectives of the work developed. In the cases discussed below the effect of RH is imposed by reducing (suddenly) the Kc value of macroparticles. This technique simulates the type of triaxial tests reported by Ortega (2010). In some of his strain controlled triaxial tests (Figure 19) samples initially dry were flooded when they reached some given strain level. The vertical strain rate was maintained and the change in vertical stress was recorded. The same technique was repeated in the numerical tests performed.

The macroparticle’s aggregate had the following properties: initial porosity = 51%; $Kc = 1 \times 10^6$ Pa√m and $1 \times 10^5$ Pa√m; $\mu = 0.93$. Uniform clump size of 14 microparticles. The confining stress was 1 MPa.

Figures 16 and 17 show the sample response for the three cases: $Kc_1 = 1 \times 10^6$ Pa√m, $Kc_2 = 1 \times 10^5$ Pa√m, and a ‘wetting’ effect when $Kc_1$ is reduced suddenly to $Kc_2$ when the vertical strain reached 5%. The sample experiences a collapse which is reflected in a sudden reduction of the deviatoric stress. Further straining, however, results in a recovery of strength. The reduction in porosity associated with this wetting is irreversible. This is shown in Figure 17, which
provides the variation of porosity during the tests simulated. Porosity increases because of dilatancy in all cases. However, wetting ($K_c$ is reduced) results in a transient reduction in porosity. The wetted sample falls into the porosity plot for the specimen having initially a reduced $K_c$ value.

Figure 18 provides additional information on the evolution of broken macroparticles. A value of $K_{c1}=1\times10^6$ Pa$\sqrt{m}$ results in a limited breakage of particles. When $K_c$ is decreased to $K_{c2}=1\times10^5$ the breakage rate increases. The sudden wetting takes the sample from the $K_{c1}$ to $K_{c2}$ curve.

Figure 19 shows the results of triaxial tests performed by Ortega (2010) on samples of limestone fragments ranging in size from 1 to 4 cm. The plot shows stress-strain curves for samples maintained at relative humidities of RH=10%; 50% and 100%. The driest sample (RH=10%) was fully wetted, once it reached a certain deformation, by means of two processes:
• Specimen flooding by liquid water. The test was then resumed (sample HR10%-Sat-Cut)
• Deviatoric stress was reduced to zero, the sample was flooded and the test was resumed again (sample HR10%-Sat-Desc)

Samples having a smaller RH are stiffer and reach higher strength. The RH=10% sample loaded and then flooded once it was at limiting conditions experienced a sudden reduction in strength which recovered in part as deformation increased. The stress-strain curve approaches now the curve for the RH=100% case.

The discrete model results in Figure 16 and the actual experiments are qualitatively similar. Matching model and experiments require an improved geometrical definition of particles, pore geometry and particle properties.

![Graph](image)

**Fig. 19.** Triaxial test on limestone rockfill. Stress-strain curve. Confining stress: 1.0MPa. (Ortega, 2010)

### 6 CONCLUDING REMARKS

A key aspect of rockfill behaviour is the particle breakage during the process of deformation under stress levels of common engineering interest. This paper presents some results of an ongoing research aimed at developing a suitable ‘particle’ method to analyze rockfill behaviour.

The computer program PFC3D (Itasca, 2008) offers the possibility of grouping individual spherical particles into bigger units (macroparticles) which may simulate the actual shape of rockfill fragments. The possibility of programming internally some relevant phenomena determining the failure (breakage) of individual macroparticles was used to build a dedicated particle-based model which attempts to reproduce real behaviour as revealed by large scale triaxial tests on gravels.

A ‘pyramidal’ macroparticle shape, made of 14 micro-spheres, was used in the results presented. Other geometries will be explored in future analyses.

The calculated effect of particle shape (to a limited extent), porosity and angle of internal friction follows a consistent pattern.

Particle breakage was related to fracture mechanics concepts. Rock toughness enters as a
natural property. Crack propagation is also controlled by the initial distribution (in the entire sample) of defects and its initial length as well as on stress intensity, current suction (or relative humidity) and time. The effect of some of these variables has been explored. It seems that the model developed has the capability of reproducing the main features of reference real triaxial tests on coarse gravels.

REFERENCES

COLLAPSE OF WET GRANULAR COLUMNS: EXPERIMENTS AND DISCRETE ELEMENT SIMULATIONS

FABIO GABRIELI*, RICCARDO ARTONI†, ANDREA SANTOMASO† AND SIMONETTA COLA*

* Dept. of Hydraulic, Maritime, Environmental and Geotechnical Engineering (IMAGE) University of Padova
via Ognissanti 39, 35129 Padova, Italy
e-mail: fabio.gabrieli@unipd.it; Web page: http://www.image.unipd.it

†Department of Chemical Engineering Principles and Practice (DIPIC) University of Padova
Via Marzolo 9, 35131 Padova, Italy
Web page: http://www.dipic.unipd.it

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Abstract. This work aims at investigating the effect of triggering and jamming due to the addition of a small quantity of fluid to the material. Collapse of dry and wet granular columns is studied both from the experimental and the numerical point of view. Wet samples of glass beads of different grain-sizes in the pendular state were packed in a rectangular box and then allowed to flow by removing a lateral wall. The dependence of the kinematics and the final state of the system on grain size and water content was particularly investigated. DEM numerical simulations were carried out in a 1:1 scale. A good qualitative agreement between experiments and DEM simulations was found with respect to the kinematic and the final slope profile. In particular, both the techniques highlight the strong effect of the liquid which decreases the run-out distance and time even for small liquid contents. This work demonstrates the suitability of the DEM approach also for the study of wet granular materials in static as well as in dynamic conditions, however it highlights that the water redistribution model is critical for the model outcome.

1 INTRODUCTION

The triggering and jamming mechanisms are of growing interesting in many fields of science: from the statistical mechanics to the geotechnical engineering, to the material science, and to chemical processes. At a micro-scale these phenomena have been studied for the link with the formation of amorphous material like glassy systems or emulsions; at
a meso-scale the interested is focused on the formation and run-out of granular flow (like landslides or controlled flows) or, in the industrial field, to the transportation an jamming of powders and grains in the process networks.

In the field of granular flows, recent research has been carried out on the collapse of granular columns, an unsteady reference problem which involves both triggering and jamming of the flow. The typical experiment is very simple: an axisymmetric or rectangular column [1, 2] is allowed to collapse by lifting respectively the containing cylinder or a containing wall. The material collapses generally evolving to a pile with a typical inclination slightly lower than the angle of repose. The position of the avalanche following triggering of the motion was usually registered in time to reconstruct the kinematics of the collapse, and the final runout distance and heap height were estimated in order to develop scaling laws for the final deposit. In the various works available in the literature, the effect of the initial aspect ratio, the size and shape of the grains, the roughness of the bottom surface was evaluated for the case of dry granular materials. For this case, discrete element simulations were also performed with different approaches (classical molecular dynamics or contact dynamics methods) generally confirming the experimental results [3, 4]. Various models have also been proposed to explain the obtained experimental data [5].

In this work research on granular column collapse is extended to the study of wet granular materials, both from the experimental and the numerical point of view. Wet granular materials are very interesting because, generally, the presence of water in the granular medium greatly affects phenomena even in very small amounts [6]. This research represents a first step in the investigation of the effect of small quantity of fluid on triggering and jamming.

In this paper the dependence of the kinematics and the final state of the system on grain size and water content was particularly investigated both experimentally and numerically (through DEM). This work demonstrates the suitability of the DEM approach also for the study of wet granular materials in static as well as in dynamic conditions, however it highlights that the water redistribution model is probably critical for the model outcome.

2 MICROMECHANICS OF WET GRANULAR MATERIALS

The degree of saturation of wet granular materials can be divided into 5 states [7]:
(1) completely dry when water content is zero, (2) pendular state when the air domain is connected and a little amount of water is shared by couples of grains forming the so called capillary bridge or pendular ring or meniscus, (3) funicular state when pendular rings collapse on one another and the water is shared by 3 or more solid grains, (4) capillary state when the liquid domain is connected and air is confined in some bubbles and (5) completely wet or saturated when the air content is zero. In this work it was chosen to focus on the pendular regime, which is usually considered to take place in the range $w = 0-5\%$, where $w$ is the weight ratio between liquid and granular material. When two particles share a little amount of fluid an attractive force exists between them. This force is due to two component namely cohesion and adhesion. The first term is related
to the liquid surface tension; the second instead depends also on the properties of the solid-liquid contact. If the particles are equal and spherical and the liquid surface is symmetrical (this is reasonably true for low Bond number and low normalized capillary volume) these force mainly acts along the direction joining two particle centers and can be very high in comparison to contact forces normally experienced at the contacts.

Following Rothenburg & Bathurst [8] and Santamarina [9], normal contact forces for a random packing of dry spheres with void ratio $e$ and coordination number $m$ can be estimated as:

$$F_{\text{cont, n}} = 4R^2\sigma_{\text{iso}}\frac{\pi(1 + e)}{m};$$  \hspace{1cm} (1)

One can observe that normal contact forces mainly depend on $R^2$ and on the depth of the particle, which mainly controls the isotropic tension $\sigma_{\text{iso}}$. On the other hand volumetrical forces (i.e. gravitational forces, unbalanced forces) depend on $R^3$ while maximum capillary forces are linearly proportional with $R$ [10, 11], as it will discussed in the follow:

$$F_{\text{cap, max}} = F_{\text{cap}}(s = 0) = -2\pi R\gamma \cos \phi$$  \hspace{1cm} (2)

Viscous forces instead strongly depend on the relative velocity between particles [12], but they can be considered really small in the study of transition phase problems (static to flowing and vice versa). In figure 1 these forces are plotted as a function of particle radius depicting which force prevails from a micromechanical point of view. This graph does not take into account fluctuations of these forces that can be very important, especially for contact forces.

![Figure 1: Typical values of different types of micromechanical forces varying particle size.](image)

It should be noted that this graph extents down to very low particle size (typically < $4\mu m$). For lower particle radii, van der Waals interaction forces are expected to prevail, but
were not taken into account in this study. Exploring the grain size of many medium-coarse granular materials (namely sandy-silty soil in geotechnics) some interesting observation can be simply obtained. Indeed, all micromechanical forces decrease with particle size but in a different manner. Contact forces prevail for larger particle size while capillary forces in this range are very low; on the other hand for lower radius capillary forces increase and overcome contact forces. Substituting some trial values of \( R \) in equation 2 and comparing the results with the weight of the particles with the same size, one can estimate the number of particles that can be assembled to form a vertical capillary chain. From this simple observation it should be stated that the maximum depth of influence of a particle with \( R = 1 \) mm at the surface of a wet granular material extends at maximum to approximately \( \sim 8R \) equal to 8 mm depth. For lower particle size \( R = 0.1 \) mm this zone extends to \( \sim 870R = 8.7 \) cm. It is clear that, in this range of grain sizes, the dynamics of wet granular materials will strongly depend on the grain size itself and on size of granulated cluster of particles.

The first solution to the problem of the capillary force existing between two spheres was developed by Haines [13] and Fisher [11] solving Young-Laplace equation for a simplified geometrical configuration: the fluid surface was approximated as a toroidal ring (see Figure 2a). Recently some authors, in order to increase the accuracy of this solution and at the same time to keep its simplicity, have provided other empirical equations based on the fitting of numerical solutions of the Young-Laplace equation for different radii, capillary volumes and gaps between particles [14, 15]. These equations represent the capillary force as a function of particle gap, contact angle and capillary volume. They obtained satisfactory results in comparison with experimental tests and allowed to extend the suitability of these equation for uneven particle size [16]. Another possible way is the use of an approximation of the so-called minimum energy approach that finally leads the following rational equation:

\[
F_{\text{cap}}(s, V) = -\frac{2\pi R\gamma \cos \phi}{1 + \left[s/2d(s, V)\right]},
\]

\[
d(s, V) = (s/2) \left[-1 + \sqrt{1 + 2V/(\pi Rs^2)}\right],
\]

where \( s \) is the gap, \( V \) is the capillary volume, \( \phi \) the contact angle, \( \gamma \) the liquid surface tension. In addition Lian et al. [17] experimentally observed that the bridge broke when:

\[
s = s_d = \left(1 + \frac{\phi}{2}\right) V^{1/3},
\]

It can be noted that \( F_{\text{cap}} \) has a maximum value when two particles are in contact \( (s = 0) \) and, in this condition, it does not depend on capillary volume. \( F_{\text{cap}} \) decreases with the gap \( s \) and the larger the volume, the higher the capillary force and the maximum allowed distance between the two particles (see Figure 2b). On the other hand, in order to form a capillary bridge a gap \( s < s_d \) is not sufficient, but it is necessary that the distance between particles is lower than:
$$s_c = \frac{12V}{\pi \left(1 + \frac{1}{1 - \cos \phi}\right)}$$  \hspace{1cm} (6)$$

![Figure 2: (a) Geometry of the capillary bridge; (b) capillary force for different capillary volumes](image)

### 3 MATERIALS AND METHODS

#### 3.1 Experiments

Experiments of granular column collapse were performed in a rectangular channel as displayed in Figure 3. The channel was made of transparent glass plates, lateral walls being 35 cm long, 12 cm high, with a gap of 5 cm between them. A 5 x 15 cm glass plate was used as the removable confining wall for the experiment. As the focus of the present work was to understand the effect of wetting on collapse dynamics, and mainly to investigate different water amounts and particle diameters, the influence of the initial aspect ratio of the column (which was studied, for the dry case, in a number of experimental and numerical works) was not addressed. The initial dimension of the column was therefore kept fixed to length $W_0=7$ cm and height $H_0=8$ cm (approximately) for all the experiments and simulations. The sample was first prepared separately by mixing a certain amount of liquid to the material, which was then poured in the experimental box. The effective amount of liquid in the material was quantified by weighing the dry, empty preparing container and the container after having poured the spheres into the column. It was important to quantify precisely the amount of water in the sample since the water involved was a very scarce quantity ($\sim 5$ mL). The experiment was performed by lifting by hand the moving wall, allowing the column to collapse freely under the action of gravity. By looking at the recorded movies, it was verified that manual lifting was sufficiently
Glass spheres in two particle sizes ($d_p = 2, 5$ mm) were used for the experiments. Given the density of glass ($\rho_p = 2532$ kg/m$^3$) and the weight of the dry sample, it was possible to estimate the number of particles in the experiments, which were nearly 41000 for 2 mm and 2600 for 5 mm spheres. Two different liquids were tested: distilled water (surface tension, $\gamma = 72.75$ mN/m, contact angle $\phi = 15^\circ$) and water with a tensioactive ($\gamma = 17.10$ mN/m, $\phi = 40^\circ$), which had the effect of lowering the surface tension of water. Contact angle measurements of the two fluids on the particles were performed by taking microscopical photos of little drops on a flat glass surface. In particular, the amounts of water tested were $w = 0$ (dry), 0.5, 1., 2., 4. %. During each experiment, the evolution of the system was tracked by taking pictures at certain time intervals using a CCD camera. In particular, two cameras were used: (1) a high-speed CCD camera (Photron FastCam PCI) capable of frame rates up to 1000 fps (which was operated at 250 fps), and (2) a high resolution CCD camera (CASIO EX-F1) which was operated at 30 fps. The first camera was employed to reconstruct the instantaneous velocity field through Particle Image Velocimetry. The second camera was employed when high resolution images were required, for example for a more accurate slope evaluation.

In order to reconstruct the instantaneous velocity field from sequences of images, Particle Image Velocimetry (PIV) analysis was employed. PIV was performed using the open source MATLAB toolbox MatPIV [18], adopting an interrogation window shifting technique [19] in three steps (24x24; 24x24; 12x12) and filtering the velocity field to remove wild vectors.

### 3.2 Numerical simulations

From the pioneering work of Cundall and Strack [20] Discrete Element Methods (DEM) were extensively used in many field of sciences. The goodness of this method was proved with respect to many quasi-static problems [21, 22] as for steady granular flows [23]. In the original form, contact is represented by a linear spring with a dashpot in the normal direction and a linear spring, a dashpot and a frictional slider in the tangential one. The
capillary force can be easily added in final form of unbalanced forces computation:

\[ m\ddot{x}_i = \sum F_{cont} + \sum F_{cap} + F_{grav} \]  \hspace{1cm} (7)

Where \( F_{cont} \) are the contact forces derived from the spring-dashpot analogical model and \( F_{cap} \) are obtained with equation 3. Another important issue regards the distribution of liquid volume. Following the evidence obtained from X-ray tomography experiments, in numerical simulations the liquid volume was equally distributed on 95% of potential contact, intending potential contact as a couple of particle that could potentially share that specific amount of volume.

The redistribution algorithm was structured as follows: when a couple of spheres sharing a meniscus detaches (when the gap \( s \) overcomes \( s_d \)) the liquid volume equally distributes on the two spheres. When a particle rotates the attached drop of liquid follows its movement, and a capillary bridge re-creates when these conditions are contemporary met: (1) the gap between the particles is lower than the formation distance \( s_c \) given in Eq. 6, and (2) the position of the drop is within a certain threshold angle from the line connecting the two spheres. For two drops to collapse to one bridge, both drops have to satisfy the requirements, otherwise at least one drop will not form a bridge.

A sample with the same geometry and dimensions, and the same number of particles of the experiments was generated and was initially prepared as a loose random packing which was then sedimented due to gravity. As the material was the same, the same contact parameters were used for sphere-sphere and sphere-wall contacts. The parameters were previously calibrated on the base of some triaxial tests at different confining stresses (normal and tangential stiffness: \( k_n = 400 \text{kN/m}, k_s = 100 \text{kN/m}; \) contact friction coefficient: \( \tan \phi = 0.62 \)). The numerical experiment aimed at accurately reproducing the experimental set-up: the lifting movement of the moving wall was imposed, as estimated from the image sequences, to be an accelerated motion with an acceleration \( a = 16 \text{ m/s}^2 \).

4 RESULTS

4.1 PIV analysis

For the experiments where image sequences were collected at 250 frames per second, it was possible to perform a particle image velocimetry (PIV) analysis to reconstruct the instantaneous velocity field. Results from PIV are reported as an example in Figure 4 for the case of dry, 5 mm particles. A complete set of PIV tests was not performed due to technical reasons, and it was preferred to concentrate the efforts more on slope profiles than on instantaneous velocity fields. The dry, 5 mm test which is analysed in the Figure is however very useful to understand some important features of the phenomenon. Future efforts will concentrate on a systematic PIV campaign.

As it can be noticed in Figure 4, where the evolution of the collapse event is shown at 4 different times, after removing the confining wall the collapse starts in the lowest part of the column, setting into motion only a part of the original sample. Indeed a zone can be
recognized where no motion occurs, which can be identified as a triangular zone close to the rear confining wall, containing nearly half of the material. Following Rankine theory, for cohesionless frictional material with friction angle $\phi$, the soil mass interested to this movement is a triangular wedge contained between vertical and an angle of $45 - \phi/2$ with respect to vertical. The collapsing material rapidly deposits forming a slope with a uniform angle.

4.2 Kinematics

The kinematics of the collapse can be appreciated by looking at Figures 5 and 6. In Figure 5, the shape of the surface during the collapsing event is tracked for the experimental data, for dry and $w = 1\%$ samples. It is clear from the figure that the shape of the sample depends only slightly on grain size, but depends strongly on the presence of water. In particular, the figure shows that according to experience, smaller particles are more affected by the presence of water: while 5 mm particles behave, wet or dry, nearly in the same way, 2 mm particles flow in a more rigid manner and with a certain delay in comparison with completely dry particles. Then the final slope has a steeper angle and the runout length is less than in the dry case.

In figure 6, the time evolution of the normalized runout distance and the normalized maximum height of the pile is described for both experiments and simulations. Experiments show the typical sigmoid profile, composed of an accelerating zone, a zone with approximately constant velocity, and a decelerating zone. The delay in the motion of the 2 mm particles is even more clear from this figure.

As reported in the literature on dry column collapse, for the dry case the particle diameter plays no role on the dynamics. Here it is demonstrated that a small water amount is sufficient to make the particle diameter play an important role, even for coarse
particles (as the 2 mm particles are).

![Graphs showing slope evolution in time for different conditions.](image)

Figure 5: Slope evolution in time for some experimental tests, extrapolated from the images at times $t = \{0\ s, 0.17\ s, 0.23\ s, 0.36\ s, 0.49\ s\}$

### 4.3 Final deposit

The strong effect of water on the behavior of the column is clear also looking at the final values of heap height and runout length shown in Figure 7. Results show how the water content plays a strong role, particularly on 2 mm spheres, and that increasing the water content the pile gets higher and shorter. The final height of the heap is nearly the same as the initial height for wet 2 mm spheres: this suggests that the swedge-shaped static zone is more extended in the wet case. Collapse experiments performed with a different wetting fluid (with a low surface tension), for 2 mm particles, were expected to display a lower cohesive behavior; results showed that little difference exists between the two wetting fluids. On this point more accurate measurements should be performed.

### 4.4 Comparison between experiments and DEM calculations

It was difficult to precisely define the end of the pile particularly at the end of the simulations because of a layer of particles rolling away near the head of the front. This phenomenon is not present in the experiments probably because of the redistribution mechanism or lower restitution of the particles. For this reason it is more reasonable to compare the kinematics in the accelerating and constant velocity regions. Regarding the
dry results, a good qualitative agreement is found. DEM predicts a similar behavior for 2 mm and 5 mm particles in the dry case. For the wet case, the heap height variation in time is reasonably reproduced in DEM simulations, and the initial delay of wet material is also observable from the results. However, the great difference in the runout length variation in time between 2 mm and 5 mm wet particles and, in general between wet and dry samples, is not evident. It can be hypothesized that this should be due to the redistribution mechanism, which is probably not efficient enough. By looking on the final profiles and their dependence on water content, at first the difficulty of estimating the runout length appears particularly on the case of 5 mm spheres. By looking at the figures representing variation of deposit height and final angle, it can be said that at least qualitatively the DEM approach captures the increasing of the heap angle with water content, and quantitatively predicts the final angle and height for the dry case. Once again DEM simulations seem to underestimate the effect of water, particularly on 2 mm spheres.

5 CONCLUSIONS

In this work experiments and numerical simulations have been presented for the collapse of dry and wet granular columns for different particle diameters. Experiments highlighted the strong effect of the addition of water on the kinematics and on the final slope profiles. DEM simulations, which employ a particular redistribution mechanism, appear to agree qualitatively with the experimental results. In order to reach a quantitative agreement, some refinements are needed probably on the redistribution mechanism and on particle restitution coefficients.
Figure 7: Experimental and numerical results obtained for different particle diameters and for different water contents: (a) Final length of the heap rescaled on initial length vs water content (b) final height of the heap rescaled on initial height vs water content (c) final heap angle versus water content.

REFERENCES


CREEP BEHAVIOUR OF CONFINED LAYERS OF POLYHEDRAL GRAINS

J.C. Quezada*, F. Radjai† G. Saussine*

*Innovation and Research Department of SNCF
45 rue de Londres, 75379 Paris Cedex 8
e-mail: juan-carlos.quezada-guajardo@sncf.fr

†LMGC, Université Montpellier II
CC048 Place Eugène Bataillon, 34095 Montpellier
e-mail: franck.radjai@univ-montp2.fr

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Abstract. By means of contact dynamics simulations, we investigate the creep deformation of a thin granular layer composed of irregular polyhedral particles under the action of a constant vertical overload applied on a horizontal wall on top of the layer. We show that the total deformation induced by the overload increases with the ratio between the vertical and confining horizontal stresses and the aspect ratio of the sample. The effect of the aspect ratio is a consequence of the mobilized wall-grain friction forces at the top and bottom boundaries, that lead to enhanced strength by stabilizing strong force chains at the center of the sample. We also evidence the influence of loading history due to strain-induced fabric change or inertial effects resulting from the instant application of the overload. The topology of the contact network evolves in close correlation with creep. In particular, the face/face contacts between polyhedral particles concentrate largest force chains and their number is an increasing function of creep. A crucial feature of a confined granular system is the statistical variability of the mechanical response that we analyzed for creep deformations by performing a large number of simulations for independent initial configurations. Our data indicate that the distribution of fluctuations with respect to the mean creep falls off exponentially.

1 Introduction

Granular media behaviour has been at the focus of several experimental studies. Examples are hopper flow, jamming-unjamming transition and granular avalanches [3, 11]. One of these phenomena is the creep in granular media under static overload. This creep involves axial deformation induced by the applied overload, allowing the system to explore
metastable configurations. This axial deformation produces in the granular material accumulated plastic deformations, know as settlement. Moreover, the mechanisms of creep in granular media are badly understood.

In many configurations, we can find a few numbers of grains in a composed layer, such as hopper flow, avalanches and railway ballast track, for example. These confined granular systems are the thin granular interfaces since its thickness is below the correlation length of contacts forces and particle displacement during a quasi-static flow [9].

In this paper, we present a numerical study of the mechanical behaviour of a confined layer under the action of a constant overload. We use the contacts dynamics method [5, 7, 2, 4, 10]. We focus on the settlement levels due to the creep deformation, under several applied overload and different initial configurations. We show the influence of the stress ratio, aspect ratio and loading history in the settlement. These results show intrinsic fluctuations, which is associated with the statistical variability of the mechanical response. Our data suggest that the distribution of mean creep fluctuations follow a decreasing exponential law.

2 Numerical Procedures

In this section, we briefly introduce the contact dynamics (CD) method with polyhedral particles as well as the numerical procedures used for the preparation of the numerical samples.

2.1 Contact dynamics method

The simulations were carried out by means of the contact dynamics (CD) method with irregular polyhedral particles [5, 7, 2, 4, 10]. The CD method is a discrete element approach for the simulation of nonsmooth granular dynamics with contact laws expressing basically the mutual exclusions and dry friction between particles without elastic or viscous regularization often used in explicit methods such as molecular dynamics or distinct element method introduced by Cundall and Strack [1]. Hence, this method is particularly adapted for the simulation of perfectly rigid particles. The nonsmoothness refers to various degrees of discontinuity in velocities arising in a system composed of rigid particles. In this method, the equations of motion for each particle are formulated as differential inclusions in which velocity jumps replace accelerations [6]. The unilateral contact interactions and Coulomb friction law are treated as complementarity relations or set-valued contact laws. The time-stepping scheme is implicit but requires explicit determination of the contact network. Due to implicit time integration, this scheme is unconditionally stable\(^1\).

At a given step of time evolution, all kinematic constraints implied by frictional contacts

\(^1\)For our simulations, we used the LMGC90 which is a multipurpose software developed in Montpellier, capable of modeling a collection of deformable or non deformable particles of various shapes by different algorithms [2, 7], see www.lmgc.univ-montp2.fr/ dubois/LMGC90.
between particles are simultaneously taken into account, together with the equations of
dynamics, in order to determine all velocities and contact forces in the system. This
problem is solved by an iterative process pertaining to the non-linear Gauss-Seidel method,
which consists of solving a single contact problem with other contact forces being treated
as known, and iteratively updating the forces and velocities until a convergence criterion
is fulfilled.

The determination of the contact set for irregular polyhedral particles proceeds in three
steps. First, a “bounding box” method is used to sort a list of neighboring particle pairs.
Then, for each pair, the overlaps are calculated through a 3D extension of the “shadow
overlap method” [2, 12]. Several algorithms exist for overlap determination between con-
vex polyhedra [8, 13]. In the case of an overlap, the contact plane is determined by means
of the intersection between the two particles. This detection procedure is fairly rapid and
allows us to simulate large samples composed of polyhedral particles.

The contacts between polyhedral particles belong to different categories, namely face-
face, edge-face, vertex-face, edge-edge, vertex-vertex, vertex-edge. The vertex-vertex and
vertex-edge contacts are rare. Face-face contacts are represented by three points, cor-
responding to three geometrical constraints, and thus will be referred below as triple
contacts. The edge-face contacts are represented by two points and will be called double
contacts. All other contacts are simple contacts represented by a single point. In the
iterative procedure of determination of the contact forces and velocities, the points rep-
resenting the contacts between two particles are treated as independent points but the
resultant of the calculated forces are attributed to the contact with its application point
located on the contact plane.

2.2 Sample preparation

We generate 32 numerical samples composed of 2700 perfectly rigid polyhedral grains.
The grain shapes are taken from a library of 1000 digitalized ballast grains\(^2\). Each grain
has at most 70 faces and 37 vertices and at least 12 faces and 8 vertices. Fig. 2 shows
several examples of the polyhedral grains used in the simulations. The size of a grain is
defined as two times the largest distance between the barycenter and the vertices of the
particle, to which we will refer as the “diameter” of the particle. The grain sizes vary
between 25 mm and 50 mm with 50% of diameter 25 mm, 34% of diameter 37.5 mm and
16% of diameter 50 mm. The bulk density of the grains is 2700 kg m\(^{-3}\). The coefficient of
friction between the grains is 0.8 for all samples. The normal and tangential coefficients
of restitution are \(\simeq 0\).

The preparation protocol consists in first pouring the grains into a cylindrical box
with zero grain-wall friction. A rigid block of weight \(W = 16\) kg is placed on top of
the sample. Then, the cylinder is removed and a radial confining pressure of 80 kPa is
applied on the sample by a uniform distribution of radial forces over the outmost grains

\(^2\)The library was provided by the French Railway Company SNCF.
located on the periphery of the cylinder while keeping the bottom plane fixed. The sample obtained by this procedure is subjected to vibrations of small amplitude by applying a vertical sinusoidal displacement on the top wall. The vibrations last for about 0.4 s with a frequency of 10 Hz. Then, the vibration is stopped and the sample is allowed to relax to static equilibrium. The resulting sample has a height of \( H_0 = 0.4 \) m and a radius of \( R \approx 35 \) cm. The applied protocol is fairly reproducible and the packing fraction \( \rho \) for the 32 samples is in the range \([0.610, 0.626]\). Fig. 1 shows a snapshot of a numerical sample.

The creep deformation is studied by applying a constant overload \( F \) on the top wall. In a series of simulations, 500 different values of \( F \) varying from 0.9 kN to 120 kN were. The deformation lasts until a stable equilibrium state is reached. The time step was 4.10^{-4} s in all simulations and at most 150 time steps were needed for full stabilization. The CPU time was 2.10^{-3} s per particle and per time step on a Dell computer of speed 3.16 GHz. The creep was also investigated by stepwise application of small overloads and with different values of a “pre-consolidation” overload; see below.

3 Creep deformation

Figure 3 shows the creep deformation \( \delta H \) of a sample subjected to different values of the overload \( F \) as a function of time. The total creep increases with \( \eta \).

The total creep deformation \( \Delta H \) depends on how the overload is applied. The same total overload may be applied in two or more steps. Let \( n \) be the number of steps. We find that \( n\Delta H(F/n) < (n-1)\Delta H(F/(n-1)) \). This implies that a quasi-staic compression of the sample should yield the lowest level of deformation. In other words, quasi-static loading provides the lower bound for creep deformation.

Fig. 4 displays the creep deformation \( \Delta H(t) \) for different stepwise applications of a total overload of \( F = 60 \) kN.

The abrupt application of an overload leads to the inertial motion of the grains. The extra inertial forces, in addition to the total force \( F + \text{top wall weight} + \text{sample weight} \) can be measured on the bottom wall.
The creep deformation depends also on the aspect ratio $\alpha = H_0/D_0$ of the sample. This is mainly due to the fact that the static equilibrium of the sample is controlled both by the internal angle of friction and the friction with the walls at the top and bottom walls (this will be analyzed below).

Fig. 5 shows the time evolution of creep deformation for different samples of different aspect ratios $\alpha$ for the same overload. Larger aspect ratios lead to larger creep deformation.

Finally, the creep deformation shows sample-to-sample fluctuations. Fig. 6 shows the time evolution of creep deformation for the same values of $\eta$ and aspect ratio $\alpha$ but for different initial configurations. The total deformation $\Delta H$ is different. The initially configurations have slightly different values of packing fraction. This difference cannot explain the large creep fluctuations.

All these data indicate clearly that the settlement due to creep deformation depends on various parameters (stress ratio, aspect ratio, loading history) and shows intrinsic fluctuations (depending on subtle details of the microstructure), which can be considered as resulting from a stochastic process.

In the following, we first consider the mean behavior by averaging over different realizations of creep deformations as a function of the stress ratio and and aspect ratio for a given protocol of loading history. Then, we focus on the fluctuations and sample-to-sample variability.

4 Parametric study

In this section, we focus on the joint effects of stress ratio $\eta$ and aspect ratio $\alpha$ on the total creep deformation.
Fig. 5 shows the total settlement $\Delta H$ as a function of $\eta$ for the same initial configuration and for $\alpha = 0.5$. We observe that $\Delta H$ increases with $\eta$ in two steps. $\Delta H$ only slightly with $\eta$ until $\eta \simeq 0.5$, then grows much faster for higher $\eta$.

The rather low creep deformation below $\eta = 0.5$ is mainly localized at the interface with the top wall where the packing fraction lower and the contact between the wall and the grains is ensured by a rather lower number of contacts. Only for $\eta > 0.5$, the deformation propagates into the bulk of the sample. This point will be analyzed in connection with creep variability below. This creep can be suppressed by pre-loading (pre-consolidation) the sample and allowing the sample to relax. Pre-loading levels out and homogenizes the interface and allows for a more uniform deformation of the sample. Fig. 7 shows the total plastic deformation as a function of $\eta$ for $\alpha = 0.5$ and after a pre-consolidation of the sample with a load of $F = 3.6$ KN. We see that the initial low creep has disappeared. This effect reflects the plasticity of the material. The pre-consolidation modifies the microstructure not only at the wall interface but also in the bulk. Beyond $\eta = 0.5$, the pre-consolidation has no effect as the microstructure does not evolve anymore with loading.

The joint effect of the stress ratio $\eta$ and aspect ratio $\alpha$ on the total creep deformation for a sample is displayed in grey level in Fig. 8. The isovalues of creep show clearly that the same level of creep deformation can be reached with a low stress ratio at high aspect ratios or with a high stress ratio at low aspect ratios.

The observed dependence of creep deformation on the aspect ratio is a consequence of friction with the top and bottom walls. The deformation of the packing can be viewed as a radial ”extrusion” of the material under vertical forcing. This radial spreading of the material causes a radial mobilization of friction that plays a major role in the equilibrium.
Figure 7: Total creep deformation as a function of $\eta$ for the initial configuration before and after the pre-loading.

Figure 8: The isovalues of total creep deformation as a function of $\eta$ and $\alpha$.

Figure 9: Radial stress as a function of the distance to the symmetry axis of the sample.

Figure 10: A snapshot of the grain stresses in a vertical section of the sample passing through the axis of symmetry.
We propose here a simple calculation of internal stresses by assuming that the friction is fully mobilized at the walls and inside the material as in the Jansen model for a silo. This model predicts an exponential fall-off of the stress components from the center of the cylindrical sample towards its periphery. Fig. 9 shows the radial stress $\sigma_{rr}$ estimated from the data as a function of the distance $r$ from the central axis. These data are in good agreement with an exponential fall-off of the stress in exception to the central part where the stresses are over-estimated.

Higher stresses at the center of the sample means that the strongest force chains occur at the center of the sample. This can be seen in a snapshot of the particle stresses displayed in Fig. 10.

5 Creep variability

In order to evaluate the variability of creep deformation, we generated 32 independent configurations of the same aspect ratio $\alpha$ by the same protocol and subjected them to 500 different values of stress ratio $\eta$. Fig. 12 shows the coefficient of variation $C_v = \langle \Delta H(\eta) \rangle / S_N(\eta)$ as a function of $\eta$. We see in that $C_v$ declines in the range $\eta \in [0, 0.5]$ and then remains almost constant. The high variability in the range $[0, 0.5]$ is related to the low values of the mean creep deformation and reflects the fact that the grain/wall interface varies statistically more in different samples than the bulk structure.

Fig. 13 shows the probability density function of the creep deformation for all samples where the deformations are normalized by the mean deformation for each value of $\eta$. The broad distribution of creep deformation declines almost exponentially above the mean. A peak occurs for a values of creep deformation slightly below the mean. This means that the most frequent creep deformation is not the mean creep. Both high creep deformations (the
tail of the distribution) and low creep deformations may occur with significant probability.

6 Fabric variables

The fabric, i.e. the spatial organization of gains and topology of the contact network, encodes most of the past history of loading. In this section, we consider the evolution of several basic fabric variables during creep deformation. These are the mean coordination number $Z$, the fractions $K_s$, $K_d$ and $K_t$ of simple, double and triple contacts, respectively, as well as the mean force carried by each type of contact. We show that creep deformation leads to hardening basically as a result of the evolution of the proportions of contact types. In particular, the fraction of triple and double contacts increases, leading to a higher force concentration, whereas $Z$ does not evolve. We also find that $K_s$ is higher than $K_d + K_t$, but $f_t$ and $f_t$ are larger than $f_s$. This means that the triple contacts concentrate force chains.

REFERENCES


INVESTIGATION OF DILATANCY IN BLOCK-STRUCTURED GEOLOGICAL MEDIUM ON THE BASE OF MOVABLE CELLULAR AUTOMATON METHOD

SERGEY V. ASTAFUROV*, EVGENY V. SHILKO, ALEXANER V. ANDREEV AND SERGEY G. PSAKHIE

* Institute of strength physics and materials science SB RAS (ISPMS SB RAS)
Laboratory of computer-aided design of materials
Akademicheskii ave., 634021 Tomsk, Russian Federation
e-mail: astaf@ispms.tsc.ru, web page: http://www.ispms.ru

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Summary. The peculiarities of dilatancy processes in block-structured media that experience nonequiaxial compression under shear deformation are investigated using movable cellular automaton (MCA) method. For a characteristic of compression nonequiaxiality (also termed the degree of constraint) a dimensionless parameter – the lateral to normal pressure ratio in the deformation plane – used. The main objective of the work is to trace the sequence in which various dilatancy mechanisms are involved in deformation depending on the level of shear stress and degree of constraint. It is shown that in the block-structured medium an increase in the degree of constraint causes the dominating dilatancy mechanism to change from slip of discontinuity surfaces to opening and expansion of pores. The dominating dilatancy mechanism changing because increasing the degree of constraint increases the threshold shear stress at which the slip is activated. Beginning with certain lateral pressures, the slip is impeded giving way to expansion of the pore space; however, the latter fails to provide so considerable volume change as the slip of contact surfaces does, and this decrease critical dilatation characteristics of the medium and, in particular, its dilatation coefficient and volume changing.

1 INTRODUCTION

It is well known fact that fragments of the Earth’s crust are in complex stress-strain state. In particular, there are areas characterized as relatively high and low levels of stress, as well as various relations between the pressure and intensity of shear stresses. So, even on a sufficiently large depth, where pressure is high, the stress distribution is strongly nonuniform [1,2]. This heterogeneity is manifested at all scales and is associated with a block structure of rocks.

One of the most important characteristics of the stress-strain state of the rock massif is the constraint, which greatly affects the intensity and the sequence of involving the mechanisms of deformation and fracture regime of the medium [3-7]. So one of the most important directions of investigation of regularities of the mechanical response of rocks is to identify the
role of constraint conditions.

Specific areas of rocks, which include areas of active faults and cracks, along with a compression undergo a significant shear deformation. Moreover, due to nonuniform distribution of the stress state in a medium value of compression of the system in different directions may vary considerably. Thus, the deformation of the shear zones, both at considerable depths, and near the surface occurs in conditions of nonequiaxial compression. Therefore, the actual problem is to study the influence of the ratio of stresses acting on the shear zone in the normal and lateral with respect to its line direction (hereinafter such a parameter called the degree of constraint of the shear zone) on the main parameters of the mechanical response of the medium [8,9].

An important factor which determines the behavior of geomedium is the change of its volume during shear deformation (dilatancy) due to the repackaging of individual fragments, as well as the formation of new or closing of existing cracks. The result of dilatancy are changing the structure of the block geomedium her wave and mechanical properties [1]. Dilatancy plays a great role in the deformation processes taking in the crust and, in particular, for earthquakes. Since it is associated with the processes of softening and hardening of rocks, it contributes to the spread of fluids in the crust, etc. [1]. In this regard, important to analyze the effect of the degree of constraint of the shear zone at its dilatation characteristics. In this case, interest is not only the phenomenon of dilatancy, but also the dependence of the involvement of different dilatancy mechanisms on the level of shear stress and the extent of damage in the medium [10].

Carrying out of full scale studies of dilatancy processes in real natural systems is extremely complex, although the problem under consideration. Therefore, important information about the behavior of fragments of rocks could be obtained based on the physical and computer-aided simulation. Note that when conducting such studies on geological materials must take into account the main features associated with multiscale hierarchical organization of the block structure [2,9,11]. In particular, the interface between structural elements in geomedium possess lower compared with blocks of mechanical properties. Therefore, the main deformation processes in rock massifs localized at interblock interfaces. Consequently, taking into account of the block structure of the medium and related geomechanical processes, in particular, the formation of discontinuities and growth of cracks at the interfaces is a prerequisite for studying the behavior of rocks in different deformation conditions. This work is devoted to theoretical investigation of the influence of a block medium degree of constraint on the dilatancy effects during shear deformation. The study was based on computer-aided simulation by movable cellular automaton method (MCA) [12,13]. This method is a type of particle-based method and a number of years been successfully applied to study the characteristics of deformation and fracture of consolidated, granular and loosely coupled geological media.

2 PROBLEM STATEMENT OF COMPUTER EXPERIMENT

As was mentioned in the introduction, to construct models of block-structured geological media must take into account the hierarchical organization of their structure. In other words, on any considered scale level it is necessary to take into account the deformation processes at smaller scales [9]. Under such a formulation of the problem of special interest to study the
general peculiarities of the mechanical response of a block medium with the so-called one-ranged structure, i.e. a medium consisting of structural elements of the same scale. Therefore, in this paper to study dilatancy process was carried out using a model system with blocks of the same size, separated by the interface region (boundaries) (fig. 1 a) [9,14]. In this case, as in [9], taking into account the higher (compared with the blocks) the extent of damage and porosity of the inter-block interfaces was carried out by setting them lower strength and deformation characteristics. Used a structural model of block medium was realized in the two-dimensional version of the method of movable cellular automata [9,12]. Calculation of stress-strain state was carried out in an approximation similar to the approximation of plane-strain state. The choice of this approach stems from the fact that it is most correctly reflects the stress-strain state of the medium at considerable depths.

In analogy with [9] for the automata modeling blocks, determined by linear response function, corresponding to high-strength materials deforms elastically (curve 1 in fig. 1 b). Response functions of the automata that simulate the interface areas were characterized by a long section, corresponding to the accumulation of irreversible deformation (curves 2 and 3 in fig. 1 b). This section of the curves simulates the effect of the processes of "destructive degradation" of the material interface (hereinafter called simply "degradation") [9]. Mechanical characteristics of blocks and interfaces (fig. 1 b) is qualitatively consistent with granite and brecciated rocks.

Higher degree of degradation of the structure and mechanical properties of the medium in the central part (core) of the shear zone took into account by assignment of low strength characteristics of inter-block interfaces in the central zone of the model sample (curve 2 in fig. 1 b) compared to the interfaces in the layers near upper and lower surfaces (curve 3 in fig. 1 b). In fig. 1 a central zone bounded by thin solid schematically by horizontal lines.

Presented model corresponds to the so-called "granular" representation of the concept of zones of active faults [15]. As noted in [9] using of this approach in conjunction with prescribed response functions of automata of blocks and interfaces allows to take into account deformation and fracture processes occurring in the medium at least on three spatial-structural levels, which can be roughly defined as micro- meso- and macroscale. This classification also applies to defects and damage in a simulated medium, which corresponds to the concept of
structural levels of deformation and fracture of solids [16]. Thus, "microdamages" can be identified as damages whose typical size is considerably smaller than the width of the interface region (which in this case corresponds to the size of a cellular automaton). The presence/occurrence of such damage is implicitly taken into account by the response function. Under the "mezodamages" in this model are the damages whose size is equal to the width of the interface zone. The presence in the original structure of interfaces of such damages took into account the assignment of pairs of unlinked automata. The formation of new "mezodamages" in the process of deformation of the samples simulated by broken of interautomata bonds in accordance with criteria similar Mises criterion. "Macrodamages" can be defined as injuries that are larger than the size of the typical structural element (in this case - the block). It should be noted that due to significant differences in the strength characteristics of structural blocks and interfaces in this model destruction process was localized in the interfacial zones. This feature corresponds to the peculiarities of the destruction of a block-structured geological media at low strain rates and moderate pressures.

Ratio of linear dimensions of the simulated region (fig. 1 a) was $L/H=5$, where $L$ - length (size in the horizontal direction), $H$ - width of the sample (size in the vertical direction). The initial stress state of the sample was set by nonequiaxial compression with forces $F_x$ and $F_y$ (fig. 1 a). The value of $F_y$ in all calculations was the same, and its specific value ($\sigma_y$) was 40% of the yield stress ($\sigma_{\text{yield}}$) of response function of the material of interfaces (curve 2 in Fig. 1b). Constrained sample was subjected to shear deformation with a small constant velocity $V_x$ (fig. 1 a). To account for inertial and dissipative properties of the simulated environment of a fragment of a block medium in the lateral surface of the sample, in addition to compressive forces $F_x$, viscous forces $F_{\text{visc}} = -\alpha V_x$ were acting, where $V_x$ - $X$ component of the velocity of the respective automaton of lateral surface.

The degree of constraint (which determines the degree of nonequiaxialty of compression) of the specimen was characterized by the dimensionless parameter $C_\sigma$, which is defined as the ratio of the specific value compresses in the horizontal direction force $F_x$ (denote it as $\sigma_x$) to the specific value of the vertical compressive force $F_y$ (denote it as $\sigma_y$): $C_\sigma = \sigma_x/\sigma_y$ [9]. Parameter $C_\sigma$ characterizes the relative magnitude of compression of system in the direction of the shear. In the paper value of $C_\sigma$ ranged from 0 to 1.

3 RESULTS OF COMPUTER-AIDED SIMULATION

As noted in the introduction, an important characteristic of the response of fragments of block-structured geological media is a change in their geometric dimensions during the deformation process, which manifests itself in particular through the dilatancy. Dilatancy of the medium depends on several factors: stress state, physical and mechanical characteristics of structural elements, regime of deformation, etc. According to [10] dependence of dilatancy strain $\Delta V$ on the shear stress $\tau$ can be expressed by a power law:

$$\Delta V \approx \delta \tau^n$$

where $\delta$ - coefficient of proportionality, $n$ - exponent, directly determines the mechanism of dilatancy. In particular, when $n<1$ is realized dilatational mechanism associated with the rotation of individual conglomerate of particles relative to each other, their relative displacement, and repackaging (i.e., this mechanism is associated with grainy/blocky structure
of the environment called sand dilatancy). For \( n > 1 \) dilatancy develops as a result of lightweight slip on the surfaces of existing or forming new cracks and pores. Following the terminology adopted in this mechanism (so-called microcrack dilatancy) is associated with behavior mesodamages at the interfaces of structural elements. "Borderline" value of \( n = 1 \) corresponds to the mechanism by which shear deformation leads to a relative displacement of individual fragments of the medium on the weak borders or large cracks (joint crack dilatancy).

Change of volume of the simulated specimen under shear loading \( \Delta V \) is due to two main mechanisms: the accumulation of irreversible strains on the block boundaries and the evolution of "mesoscopic" discontinuities [9]. Elastoplastic deformation of the interfaces could lead to a change in their width, as well as localized shear of blocks (due to the mechanism of joint crack dilatancy). Used in the calculation model of the response of movable cellular automata suggests that their forming is not accompanied by an irreversible change of volume. Therefore, extension of the model shear zone is associated mainly with mesodamages and is determined by action of two factors (hereinafter also called mechanisms): disclosure of discontinuities (increasing the "porosity") and lightweight slip along surface of damages on the block interfaces. Thus, using the developed model in our simulations make it possible to analyze the dilatancy effects associated with the block structure of the medium.

Figure 2 shows a graph of changes of the volume of the model system \( \Delta V \) from the level of shear stress \( \tau \). The value of \( \Delta V \) is defined as the relative change of volume of the specimen: \( \Delta V = (V - V_0)/V_0 \), where \( V_0 \) - volume of the simulated specimen at the beginning of shear deformation, \( V \) - the current value of the sample. Shear stress \( \tau \) in figure 2 (defined as the specific resistance force to shear deformation of the modeled system) is given in dimensionless form, obtained by normalization of its absolute value on the shear strength of "not constrained in the horizontal direction specimen (at \( \sigma_x = 0 \) The analysis of the \( \Delta V(\tau) \) curves, corresponding to different degrees of constraint of the specimen (different values \( \sigma_x \)), showed that they have a two-stage character (fig. 2). The selected stages are largely associated with the major stages of the force response of the model system (quasielastic (I) and quasiplastic (II) stages of the diagram of the shear loading in fig. 3). It should be noted that in figure 3, the shear deformation (shear angle \( \gamma \)) was defined as \( \gamma = d_y/H \), where \( d_y \) - the relative displacement of the upper and lower surfaces of the sample in the horizontal direction (fig. 1 a), \( H \) - height of the specimen.

Comparison of figures 2 and 3 shows that at the stage of quasielastic response of the shear zone (\( \tau < 0.75 \), stage I in fig. 3) curves \( \Delta V(\tau) \) have almost a linear form (stage I in fig. 2 a). With further increase of shear stress \( \tau \), in the transition region to quasiplastic response, character of the changes of \( \Delta V \) became nonlinear (phase II in fig. 2 a). These peculiarities of system behavior reflect the sequential involvement of different strain (and dilatancy) mechanisms. At a low level of the shear stress evolution of constrained medium occurs mainly by means of the relative movement of block conglomerates on some weak interfaces. This is accompanied by a small (about 0.003 - 0.004%) linear increase of the volume of the specimen (fig. 2 b). The small deviations of the character of the dependences at this stage from linear form, are apparently associated with partial repackaging of fragments of the medium. Thus, at the initial stage of loading localized shear of blocks is dominant dilatancy.
mechanism (which corresponds to (1) with parameter $n$ close to unity). The involvement of this mechanism at the early stages of deformation (in the region of the quasielastic response of the medium) is due to the fact that the sample is preloaded and the stress state of a number of inter-block interfaces is close to the yield stress to the moment of application of shear loading. Further increase of the level of shear stress (moving to the area of quasiplastic response for $\tau>0.75 \div 0.8$, fig. 3) leads to an increase of the volume fraction of interfaces, whose stress state exceeds the elastic limit and, consequently, to intensifying of the process of localization of irreversible deformations in the most stressed parts of interfaces. As a result, the sample begin to accumulate mesodamages, which become an additional source of dilatancy, whose contribution increases with their number $N$ (resulting in a ratio (1) the parameter $n$ is greater than one). Thus, in the area of transition from quasielastic to quasiplastic response of the simulated block medium there is a change of the dominant dilatational mechanism from localized shear to the mechanism of evolution mesodamages. Figure 2 a also shows that the main contribution to the total volume changing makes mesodamages as deformation mechanisms of a relatively high scale level. This relates in particular to the fact that the quasielastic stage of shear loading irreversible deformation can accumulate on a relatively small number of interfaces. Consequently, the contribution from the mechanism associated with localized shear of blocks along the weak boundaries in the first stage of deformation to the total dilatancy is negligible.

As can be seen from figure 2 a the change of volume to the moment of reaching of the ultimate state of shear zone (this characteristic is denoted as $\Delta V_c$) is determined by the degree of constraint (by the parameter $C_\sigma$). Thus in Figure 4 a shows a dependence of $\Delta V_c$ on the degree of constraint. It is seen that the curve $\Delta V_c(C_\sigma)$ has a pronounced nonlinear threshold character. Thus, in the interval $0<C_\sigma<0.4$ ultimate magnitude of change of volume increases (with a maximum at 0.4). Further, with increasing of degree of constraint ($C_\sigma>0.4$) parameter $\Delta V_c$ begins to decrease monotonically.

In mathematical models of geomedia dilatancy characterized by a number of
characteristics, the most common of which is the coefficient of dilatancy $\lambda$. In general, it is determined by the ratio of the rate of irreversible change of volume of the medium to the intensity of plastic deformation. By analogy with this parameter in the paper was introduced the "ultimate coefficient of dilatancy" $\lambda_c$, which was calculated by the ratio of the ultimate volume change $\Delta V^c$ to the angle of shear at the time of achieving of the maximum shear resistance force $\gamma^c$ ($\lambda_c = \Delta V^c / \gamma^c$). As shown in figure 4b the dependence of $\lambda_c(C_\sigma)$ is similar to the dependence $\Delta V^c(C_\sigma)$, with a peak at $C_\sigma \approx 0.4$. Note that the parameter $\lambda_c$ can be interpreted as some effective rate of change in volume of the shear zone at a constant strain rate.

![Graph of characteristics](image)

**Figure 3.** Graphs of dependences of shear resistance force of simulated system ($\tau$) on value of shear strain ($\gamma$): 1 – $C_\sigma = 0$; 2 – $C_\sigma = 0.5$; 3 – $C_\sigma = 1$. Roman numerals I and II denote quasielastic and quasiplastic stages of loading diagrams.

![Graph of characteristics](image)

**Figure 4.** Graphs of dependences of relative changing of volume of the specimen $\Delta V^c$ (a) and dilatancy coefficient $\lambda_c$ (b) to the moment of reaching of ultimate state of the system on parameter $C_\sigma$.

As was noted above, the main contribution to the change of the volume of the modeled system make the mechanism of dilatancy associated with evolution of existing and newly formed mesodamages at the interfaces of structural elements. Its effect on increasing of volume is due to the influence of two basic mechanisms described above (increases porosity and sliding of contact surfaces mesodamages). In the initial stress state the samples which are characterized by different values of $C_\sigma$, the amount of damages is almost identical, so the dependence of $\Delta V^c(C_\sigma)$ is determined mainly by the number and evolution of mesodamages.
formed during specimen deformation. Figure 5 shows a graph of the number of mesodamages $N^c$ to the moment of achieving of the ultimate state of the specimen on the degree of constraint. It is seen that in the region $0<C_\sigma<0.4$ the value of $N^c$ increases and then saturates. Consequently, the increase of volume of the model shear zone at small values of $C_\sigma$ ($C_\sigma<0.4$) is associated with an increase of the number of mesodamages. At the same time, when $C_\sigma>0.4$, where the amount of accumulated damage, at least, not decreasing, dilatational characteristics $\Delta V^c$ and $\lambda^c$ undergo reduction up to 5-7 times.

Figure 5. Graph of dependence of value of accumulated mesodamages $N^c$ to the moment of achieving of ultimate state of the specimen on the parameter $C_\sigma$.

As shown by detailed studies, the effect of a significant decrease of dilatancy at $C_\sigma>0.4$ is associated with a change of the contributions of the elementary mechanisms of evolution of mesodamages. This can be illustrated by the graphs in figure 6, which shows the dependence of the total volume changes $\Delta V$ (curve 1), free volume $V_{free}$ (curve 2) and the amount of accumulated mesodamages at block boundaries $N$ (curve 3) on the shear stress level of the modeled system $\tau$. In the calculations, the value of free volume $V_{free}$ estimated through the volume of voids ( pores). Based on the analysis of dependencies following conclusions could be made. Thus, the increase of the number of generated mesodamages accompanied by an increase of free volume value $V_{free}$. At relatively low values of $\tau$ increase of the specimen volume ($\Delta V$) is achieved by the disclosure of damage (increase $V_{free}$), as evidenced by the coincidence of curves 1 and 2 in fig. 6. However, from a certain point (point D in fig. 6 a-b), curve 2 begins to fall behind the curve 1, and to the moment of reaching the ultimate state values $\Delta V$ and $V_{free}$ may differ by several times. This means that at high shear stresses close to the shear strength of the medium, the main contribution to dilatancy makes slip along the surfaces of formed mesodamages. Formally, the threshold stress at which changing of the dominant mechanism of dilatancy takes place could be characterized as a stress of activation of mechanism of the shear slip. The difference between the total volume changing and the maximum free volume $V_{dev}$ determines the contribution to the dilatancy of slippage. As can be seen from fig. 6 a-b, with increasing of degree of constraint there is a shift of D point toward larger values of shear stress, and the value of $V_{dev}$ decreases. In the extreme case (for large values of $C_\sigma$) all the curves behave in consistently, and the values $\Delta V^c$ and $V_{free}^c$ are the same (fig. 6 c). Thus, with increasing degree of constraint contribution of the mechanism of shear-
slip along the surfaces of mesodamages decreases and at \( C_\sigma \to 1 \) becomes negligible. In these circumstances, the decisive role plays the increasing of the porosity of the medium.

![Graphs](image)

Figure 6. Graphs of dependences of volume changing (\( \Delta V \)), free volume (\( V_{\text{free}} \)) and number of mesodamages (\( N \)) on value of shear stress \( \tau \): a) \(-C_\sigma=0\); b) \(-C_\sigma=0.4\); v) \(-C_\sigma=1\).

Figure 7 shows the dependence of the specific force of resistance shear deformation at the time of activation of the shear slip \( \tau_{\text{dev}} \) and the magnitude of the difference between the ultimate values of the total change of the volume and free volume (\( V_{\text{dev}} \)) on the parameter \( C_\sigma \). As seen from fig. 7 a, with increasing of degree of constraint threshold of activation of the mechanism of slipping shifted to higher values of shear stresses and reaching saturation at \( C_\sigma \sim 0.4 \). The relative contribution of the slippage (defined, for example, in terms of the \( V_{\text{dev}} \)) grows and at \( C_\sigma \sim 0.4 \) reaches a maximum (fig. 7 b). Note that in this range of \( C_\sigma \) observed increase of the total volume changing \( \Delta V \) (fig. 4 a). Further, with increasing of parameter \( C_\sigma \) (\( C_\sigma > 0.4 \)) dependence \( V_{\text{dev}}(C_\sigma) \) decreases sharply and at \( C_\sigma \approx 0.65 \) falls to zero. Thus, if \( C_\sigma > 0.4 \) the contribution of the slippage to the dilatancy of a block medium is reduced, and at high degrees of constraint change of volume of the simulated system is provided, mainly due to the disclosure of existing and newly formed mesodamages. This leads to decrease of dilatancy of the medium (fig. 4).

Thus, the increase of the magnitude of the dilatancy \( \Delta V \) and the coefficient of dilatancy \( \lambda^e \) at low degrees of constraint \( (C_\sigma < 0.4) \) is provided firstly by the increasing role of slip along the surfaces of mesodamages. With increasing of shear stress level realization of this mechanism becomes more and more difficult, and the primary role begins to play the expansion of damages and pores.
4 CONCLUSIONS

The results of computer simulation of the shear deformation of the block-structured model specimens of the geological media in conditions of nonequiaxial compression showed that the main source of dilatancy of the medium is process of evolution of mesodamages originally existed, and the newly generated at the interfaces between structural elements. The change of volume of a block medium under shear loading is determined by the action of two elementary dilatancy mechanisms: the opening of discontinuities/pores and sliding along surfaces of mesodamages.

Analysis of the obtained results showed that the main dilatancy characteristics of the medium, in particular, the changing of volume at the time of reaching the ultimate state of the system and the corresponding coefficient of dilatancy, largely depend on the ratio of lateral and normal pressures acting on a fragment of the shear zone. At the same time dependence of these parameters on the degree of constraint have a pronounced nonlinear threshold character. This is due to the fact that with increasing of degree of constraint a changing of the dominant dilatational mechanism takes place.

Thus, with increasing of parameter $C_\sigma$ from zero to a certain threshold value (in this case $C_\sigma \approx 0.4$), the contribution to dilatancy of the mechanism associated with the sliding along surfaces of the initial and formed mesodamages increases. This is accompanied by a significant (up to 2 times) increase of the values of the fundamental dilatancy parameters. Slip along surfaces of mesodamages is a deformation mechanism with a relatively high threshold stress of activation, and this threshold value significantly increases with increasing of $C_\sigma$ (fig. 7). Because if $C_\sigma > 0.4$ a reduction of the shear strength of the medium [9] takes place, dilatational mechanism of slippage is involved in all the later stages of loading (this effect is obviously connected with the difficulty of the local shift in conditions of strong lateral compression). In this regard, contribution of this mechanism to the change of volume of the medium reduces and at the main dilatancy mechanism becomes the mechanism associated with the extension (opening) of discontinuities, which is characterized by a lower threshold of activation. However, the expansion of pores has not being provided such a large volume changing of geomedium, so that there is dependencies $\Delta V^c(C_\sigma)$ and $\lambda^c(C_\sigma)$ decrease (fig. 4).
So, in the pursuit of stress state of the block-structured heterogeneous medium to the condition of equiaxial compression hampered the involvement of dilatational deformation mechanisms and high scale levels (mechanisms with a high threshold of activation), which ultimately leads to a decrease of basic dilatational characteristics of the medium.

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SIMULATION OF CLAY SOIL DE-COMPACTION BY SUBSOILING PROCESS USING DISCRETE ELEMENT METHOD

ELVIS LÓPEZ BRAVO*, ENGELBERT TIJSKENS†, MIGUEL HERRERA SUÁREZ* AND HERMAN RAMON*

*Division of Mechatronics, Biostatistics and Sensors (MeBioS), Department of Biosystems, Faculty of Bioscience Engineering, Kasteelpark Arenberg 30, B-3001 Heverlee, Belgium. e-mail: elvislb@uclv.edu.cu
†Department of Agricultural Engineering, Faculty of Agricultural and Animal Sciences, Central University “Marta Abreu” of Las Villas, Villa Clara, Cuba.

Key words: Tillage, Soil simulation, Shear test, Friction angle, DEM.

Abstract. High pressures on the soil surface by action of heavy machinery and tillage process cause soil compaction and hardpan layers formation. De-compaction is a energy demanding operation applied to break deeply compacted soil for agricultural uses. Three dimensional simulations of soil decompaction are presented based on a soil-tool interaction model implemented in DEMeter software. Formulation of soil-soil and soil-tool interaction are combined into an elastic-plastic particle based model for soil deformation and evaluated in different tension states among soil particles; The macromechanical input parameters include: adhesion, friction, Young’s modulus, Poisson’s coefficient, elastic limit, plastic limit and soil density. Compression triaxial tests and shear box tests were carried out in order to obtain the required mechanical properties for a tropical clay soil. Simulations of unconfined compression tests using different particle sizes and inter-particle tension were used to calibrate the model to experimental stress-strain curves. The performance of complex tillage tools geometries is tested with 3D simulations and evaluated based on the reaction force on the tool as a function of time and displacement. The results show qualitative and quantitative adjusts of real patter of soil behaviour.

1. INTRODUCTION

Tillage tool geometry is an important element on the integrate system for soil conservation practices. The quality of the implement to remain the crop residues on the soil surface, making limited disruption and keeping on the upper layer the organic matter is the way to avoid soil degradation by erosion, Carbon releasing and soil compaction. Mulch tillage, ridge tillage, zone tillage and no-tillage are some of the principal types of conservation tillage techniques, its purpose is to reduce tillage operation focus in economic and environment advantages, improving soil quality, time and energy reduction [1]. Several effects of conventional tillage based on soil inversion, as a moldboard plow, become soil more susceptible to erosion, reduce bio-organisms diversity and contribute to hardpan formation.

Spatial soil redistribution during tillage depend basically on particular characteristics of the implement used, this translocation increase for moldboard conducted in down slope
direction [2]. Soil physical and chemical degradation including soil compaction, organic matter losses and nitrogen deficiencies is more pronounced with conventional disk tillage than conservation tillage; evaluation of chisel plow, no tillage and flexible tillage showed the tillage system effect on soil quality indicator [3]. Enhance soil organic Carbon stabilization in tropical soil is affected mainly by tillage disturbance, consequence of to apply long term of soil preparation with ripping tools for sandy and clay soil, residue retention and reduction tillage decrease the organic Carbon decomposition[4].

Agricultural subsoiler is a tillage implement used to working in deep layer of soil, in the beginning designed to break up the hard soil layers and uniform compaction, the non-inversion property agree with low-till practices under conservation tillage criterion. As a result of transition from moldboard plow to vertical tools, many implements had been testing on different soil and crops plantation in order to minimize soil and mulch disturbance, soil properties and crop particularities need to be manages carefully to warranty positive effect from new tools geometries on tillage operation [5]. Soil type is considered the main factors for successful adoption of non-inversion, relatively well suited for clay soil, conservation tillage reduces the risk of hard seedbed formation, however for some sands with angular structures the tillage exclude air and water movement [6].

Between soil physical properties and tillage tools geometry exist a close relationship determining the proportion of soil disturbance during the process, optimization of tillage tools focusing in geometrical modification had been making on moldboard plough obtaining significantly draft reduction requirement [7, 8]. Field performance of implement for future application on soil-ecosystem had been evaluated in nineties decade, testing several variant of tool shape, speed and draft force, equipments for conservation tillage were evaluated at the farm level correlating energy and seedbed quality [9].

Data from field and soil lab experiment has been compute using mathematical models offering more accurate, faster and extended prognostic of soil behavior. Computational techniques as well as finite element methods (FEM), discrete element methods (DEM), artificial neural network (ANN) or computational fluid dynamics (CFD) are indistinctly used with different purposes allowing to pass from quasi-static to dynamic soil analysis on the rheological behavior of soil [10]. FEM models to simulate runoff process from agricultural land with reasonable good agreement between simulation and experimentally test predict the effect of water flow, topographic condition and crop parameters [11]. Considering the soil as a continuum medium, several constitutive models has been creates and improved focused on capturing the particular soil behavior, this models dependent mainly on elastic and plastic deformation. Modified Cam-Clay model was implemented with the object to derive time dependent effect taken accounts the effect of anisotropic and expansion of loading, affected by the principal stress redirection, the validation of the simulation was carried out using undrained shear box and creep test [12]. Draft forces simulation by FEM were conducted using different tools geometries on two and tree dimension with the aim to investigate the effect of cutting speed and cutting angles in draught force requirements during soil-tool interaction [13-18].

Related with the limitation to apply FEM to simulate the granulated medium, DEM is applied to resolve the dynamic process showing a extend field for soil application. Particles interaction on DEM shows a close similitude with soil mechanical contacts take place between real grains, this contacts also exist and can be calculated between tool and soil, many
contacts models rules the behavior of overall simulation depending on the nature of the element that interact with others, the overlapping among elements is the key for contact resolution, geometrical information is provided from two element in contact obtaining velocity and position vectors, tangential and normal forces is computed and contact forces for all particles in each time step[19]. Methodology to obtain the micro mechanical input parameters for DEM based on in situ field tests, showing a well correlation before optimization between real and simulation deformation curve [20]. Simulation of soil-tool interaction with high rate of plastic deformation was modeled using wide cutting-blade and soil particles conformed by clumps of two disks with cohesion forces, DEM result were evaluated for two dimension different blade shapes, the effect of soil flow in front of the blade was related with horizontal and vertical forces [21].

The objective of this work is to implement a DEM model in order to simulate the draft force requirements during soil tool interaction for decompaction and non inversion tillage on different physical condition in a tropical clay soil.

2. MATERIALS AND METHODS

2.1 Model description

Classical DEM model proposed by Cundall and Strack [19] was used to compute the interaction between soil particles and tillage tool, two kinds of contacts were implemented: soil-soil and soil-tool, for both calculation was applied the same contact scheme varied only on mechanical properties input. The model dealing with the system forces composed by: normal, shear, gravity, adhesion and friction force (Fig. 1), the friction force is applied only during sliding when shear force is bigger than Coulomb friction criterion.

Based on soil macro-properties the micro-properties were dynamic calculated using the geometrical parameters obtained from particles interaction in each time step. Force in normal direction is calculated by:

\[ F_n = kn\Delta u_n + \eta_n \left( \Delta u_n / \Delta t \right) \]  

(1)

Figure1: Force system applied for simple contact point between two particles. \( F_f \): Friction Force, \( F_{coh} \): Cohesion force, \( F_n \): Normal Force, \( F_s \): Shear Force, \( F_g \): Gravity Force.
Where $kn$ mean normal spring, $\Delta u_s$ is the variation of normal overlapping, $\eta_s$ viscous damping and $\Delta t$ time step variation. Equation for normal spring [22] enclose the relationship among elastic properties and dimensional data as:

$$kn = \frac{E_{ab}A_{int}}{D_{eq}^{ab}} [1 + \frac{\alpha_k}{\beta_k (1 + \nu) + \gamma_k (1 - \alpha_k)]}$$

(2)

Where $E_{ab}$ is the equivalent Young’s modulus of the two contact elements, $A_{int}$ is the interior area of the contact and $D_{eq}^{ab}$ is the equivalent distant between objects, another part of the equation is the relation between poison’s ratio $\nu$ and fitting parameters [23].

Force in tangential direction is calculated by:

$$F_s = ks\Delta u_s + \eta_s \left(\Delta u_s / \Delta t\right)$$

(3)

Where $ks$ is the shear spring, $\Delta u_s$ is the variation of tangential overlapping and $\eta_s$ is the viscous damping in tangential direction.

Value of $ks$ depend of $kn$, obtained by:

$$ks = kn \left(\frac{1 - \alpha_k \nu}{1 + \nu}\right)$$

(4)

Viscous damping in normal and tangential direction is determined by:

$$\eta = \beta 2 \sqrt{\frac{m_a m_b}{m_a + m_b}}$$

(5)

Where $\beta$ is viscous damping coefficient; $m_a$ and $m_b$ were the mass of two objects in contact.

Cohesion force only act during compression in normal direction, adding its value to the total force summation of the contact. The attraction between objects increase together increment of overlapping, resulting on a equilibrium point where repulsion and attraction forces sum is zero forming a bilateral bond, to break this inter-particles bond the overlapping need to become lower than Cauchy strain of soil where the effect of adhesion force is cancelled. Force of cohesion [21]is obtained by:

$$F_{coh} = \frac{\Delta u_s c (\tan \phi \mu)^{k4}}{k3}$$

(6)

Where $c$ is macro cohesion between two objects in contact obtained by lab test, $\phi \mu$ is micro-friction coefficient, $k3$ and $k4$ are adjusted parameters related with statistical regression particular for soil material.
2.2 Virtual model implementation

Graphical interface and mathematical model formulation was implemented using the facilities of DEMeter Software developed by research particles group from KUleuven University, Belgium. Simulation was divided in two step: Fixed model with triaxial test and soil-tool dynamic interaction.

The influence of particles sizes was evaluated simulating a triaxial unconfined compression test, spherical particles with radius at 0.6, 1.8 and 2.3 mm form a cylindrical specimen with 50 mm diameter and 100 mm high, joined by cohesion forces, this sample was obtained pressing the hole particles into the void cylindrical cavity. Constant press velocity at 1m/min was used for all simulation applied on top of the sample (Fig. 2a).

![Figure 2](image_url)

*Figure 2:* Sample for unconfined compression test simulation (a); construction procedure for virtual block of soil.

The second step was the construction of virtual block of soil formed by 40,000 spherical particles generated in hexagonal compacted array and submitted to free fall inside the 650 x 400 x 300mm rectangular box (Fig. 2b). Size particles were distributed in three different layers with radius in the button between 8-10 mm, center of 6 – 5 mm and top 4.5-4 mm. All simulation was running with constant velocity of 2 m/min.

Tillage tools were designed reproducing four different geometries of subsoilers (Fig. 3), The scale of 3:1 to respect of real dimensions was used. Non soil inversion was adopted to select the geometrical parameters.
Simulation of soil-cultivator was running in three soil stage combinations; different water contents and soil bulk densities were using to obtain soft-wet soil (30% water content and 1.1 g/cm³), friable soil (18% water content and 1.2 g/cm³) and hard-dry soil (10% water content and 1.4 g/cm³). Chisel subsoiler and knife subsoiler were running in the same hard-dry soil condition to compare the draft force demanding in both cases. For the last soil-tillage simulation was added the lateral cutting knife forming a combined subsoiler (Fig. 3 d), forces demanded in hard-dry soil and soft soil with hardpan at the bottom were plotting.

2.3 Lab experiment and soil selection

Triaxial undrained compression test and shear box test were carried out in order to obtain the mechanical properties selected as macro-properties in DEM model. Elastic Young’s Modulus, internal friction, metal interface friction, cohesion and adhesion of soil were calculated as a function of dry bulk density and gravimetrical water content measured as a percentage of dry weight. Physical properties and granulometric composition (Table 1) show the high content of clay for the three principal layers becomes soil a cohesive material, the uniformity constitution on the hole depth allow to classify as a Vertisol according to the international classification based on the soil taxonomy.

Table 1: Vertisol soil properties. PL, LL and PI are the plastic limit, liquid limit and plastic index in %. Gs, specific gravity.

<table>
<thead>
<tr>
<th>Depth, cm</th>
<th>Gs</th>
<th>PL</th>
<th>LL</th>
<th>PI</th>
<th>Sand</th>
<th>Silt</th>
<th>Clay</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>2.6</td>
<td>18.6</td>
<td>63.5</td>
<td>44.9</td>
<td>7</td>
<td>27</td>
<td>66</td>
</tr>
<tr>
<td>30</td>
<td>2.64</td>
<td>28.6</td>
<td>78.9</td>
<td>50.3</td>
<td>6</td>
<td>29</td>
<td>66</td>
</tr>
<tr>
<td>50</td>
<td>2.62</td>
<td>17.2</td>
<td>67.9</td>
<td>50.7</td>
<td>8</td>
<td>29</td>
<td>63</td>
</tr>
</tbody>
</table>
Three level of soil dry bulk density ($\gamma$) were selected to capture the variability of soil compaction, values at 1.0, 1.2 and 1.4 g cm$^{-3}$ represent loosen, medium and compacted soil. Five experimental point were using to measure the influence of water content (wet) at 15, 18, 20, 25, 35 %. Factorial experimental design to predicting the behavior of above five dependent variables with respect of dry bulk density and soil moisture was preformed resulting on 60 randomized runs for triaxial and shear test, pressures at 50, 70 and 100 kPa were applied in each test to get the relation between normal stress and shear stress at failure. Multiple regression statistical analysis showed a predictable behavior of selected soil mechanical properties, statistical equation (table 2) allow to calculate the prognostic properties values with more than 94% of confidence level. The statistical equations were using by the DEM model to initialize the macro-mechanical properties input according to desire physical soil condition.

Table 2: Regression equation for soil mechanical properties.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Unit</th>
<th>Equation</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>$d$</th>
<th>$R$ %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus</td>
<td>kPa</td>
<td>$B = a + b \gamma + c \text{wet}^2 - d \text{wet}$</td>
<td>82.1</td>
<td>89.8</td>
<td>0.15</td>
<td>10.3</td>
<td>95.2</td>
</tr>
<tr>
<td>Shear strength</td>
<td>kPa</td>
<td>$T = a - b \text{wet} + c \gamma + d \text{wet}^2$</td>
<td>216</td>
<td>229</td>
<td>164</td>
<td>5.9</td>
<td>94.5</td>
</tr>
<tr>
<td>Soil cohesion</td>
<td>kPa</td>
<td>$coh = a + b \gamma + c \text{wet}^2 - d \text{wet}$</td>
<td>105</td>
<td>115</td>
<td>0.2</td>
<td>12.3</td>
<td>95.3</td>
</tr>
<tr>
<td>Soil adhesion</td>
<td>kPa</td>
<td>$adh = a + b \gamma + c \text{wet}$</td>
<td>-13</td>
<td>8.5</td>
<td>42</td>
<td>-</td>
<td>96.7</td>
</tr>
<tr>
<td>Soil friction</td>
<td>kPa</td>
<td>$f_s = a + b \text{wet} + c \gamma + d \gamma^2$</td>
<td>22.1</td>
<td>0.5</td>
<td>37.5</td>
<td>16.4</td>
<td>94.3</td>
</tr>
<tr>
<td>Metal friction</td>
<td>kPa</td>
<td>$fm = a + b \ln(\text{wet})$</td>
<td>-23.6</td>
<td>12.9</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3. RESULTS AND DISCUSSION

3.1 Triaxial unconfined compression test

The increment in the amount of particles in the same sample dimensions for unconfined triaxial test simulation, reduce the force oscillation effect during vertical wall displacement due to the increment on the contact area, particles accommodation in the void spaces reduce tension during compression increase, the magnitude of this reduction depend on the value getting for the overlapping become lower for small particles sizes, however small particles radius increase computation time due to the needed to reduce time step. Volumetric relation between sample dimensions and particles radius at 0.6 mm suggest 1:5000 units. Moreover the proximity of median soil granular distribution of the sample with minimum size particle tested suggest the optimum value proportional of minimum grain formed after soil failure.
3.2 Cultivator on three soil condition
Comparison among draft forces on cultivation process (Fig. 5) for soft-wet, friable and hard-dry soil show the average increment of 0.25 kN for each soil condition. Smaller values of resultant forces correspond with soft-wet condition on soil as a result of reduction in soil cohesion and friction coefficient. Inversely the higher forces values were reach for hard-dry soil condition according to the increment on mechanical stiffness of the soil.

The increment in force fluctuation for hard-dry soil was observed, that behavior can be attributed of the relationship between highs values of inter-particles bound and the amount of particles bond broken at the same time, however smooth curve is obtained in opposite condition tended to be linear during 200mm to 500 mm of displacement. Plastic flow characterize the soil movement patter on wet condition while fragile patter was more

Figure 4: Variation of deformation curve for different particles radius during simulation

Figure 5 Displacement of cultivator tool on soft, medium and hard soil condition.
representative on hard soil distinguished by clods formation and keeps the shape of the tool into the soil.

3.3 Subsoilers soil simulation

The draft forces needed to move the tools through the soil in hard-dry condition during simulation (Fig. 6) show a close values for tools without lateral knife (Fig. 7a, 7b), however small increment for knife subsoiler denote the influence of cutting angels, this parameter is different in both cases. Forces values obtained from the simulation have consistence with the result obtained by Sahu, R. K. & Raheman, H. (2006a) empirical equation to predict tillage draft for narrow tools according soil condition.

![Figure 6: Draft force for subsoiling with different tools geometries on hard soil condition.](image)

The energy demanded on soil decompaction increase related with the tool geometry, for combined subsoiler (Fig 7a) that increment correspond with the addition of lateral knife, moreover the work done for this tool is bigger than the other in the specific disturbed area denoting advantage in term of specific draught demanding.

No significant differences were found in the simulation of hardpan and hard soil decompaction process. Identically tool geometry in two different soil unhealthy conditions for plant production result on approximated the same draft force to pass the subsoiler through the soil. From the force demanding point of view hardpan decompaction meaning the same thing that hard soil tillage, the force needed to work above hardpan decreases according to stiffness reduction making easy the seed bed preparation but tine pressure on the bottom compresses the soil below resulting on hardpan reinforcement.
4. Conclusion

- Triaxial compression test and direct box shear, combined in experimental soil condition, provide a set of statistical equation able to predict the basic soil mechanical properties needed to implement the computation model for soil tillage simulation.
- Granular nature of soil allows simulating by Discrete Element Model tillage operation, making possible to measure the draft forces and soil loosening pattern in different physical condition of cohesive soil.
- Small particles radius reduce the oscillation force effect during simulation of unconfined triaxial compression test, however the small particles sizes need the reduction in the time step with the consequently increment on computational cost.
- Soil tillage simulation by cultivator tool in soft, friable and hard soil condition showed the dependence of draught force on dry bulk density and water content, for the case of hard dry soil maximum values of force was measured.
- Geometry changes in the subsoiler design implied variation on draft forces, however the use of lateral knife increase the area of soil disruption without proportional increment on force demand.
- Scarification treatment to break up the hardpan demands the approximate same energy to till a fully compacted soil, however further investigation in lab and field condition to measure the draft forces and soil behavior is needed to validate the tillage simulation.
REFERENCES


BREAKAGE OF NEEDLE-SHAPED PARTICLES IN A COMBINATION OF COMPRESSION AND SHEARING STRESS FIELD

ZDENĚK GROF*, FRANTIŠEK ŠTĚPÁNEK* AND PAVOL RAJNIK†

*Department of Chemical Engineering, Institute of Chemical Technology, Prague Technicka 5, 166 28 Praha 6, Czech Republic
e-mail: zdenek.grof@vscht.cz, www.vscht.cz/

†Merck & Co., Inc., West Point, PA, USA

Key words: Granular Materials, DEM, FEM, Contact Problems

Abstract. In-silico experiments of needle-shaped particles breakage during shearing have been carried out using DEM simulation. Results of preliminary studies with variation of individual particle strength, compaction ratio, and shearing rate are presented.

1 INTRODUCTION

Needle-shaped crystals are a common occurrence in many pharmaceutical and fine chemical processes. Even if the particle size distribution (PSD) obtained in a crystallisation step can be controlled, further fluid-solid separation steps such as filtration, filter washing, drying and subsequent solid handling can often lead to uncontrolled changes in the PSD due to breakage. Population balance modelling is a common method able to describe PSD changes, however two material- and stress-field specific functions are needed: the breakage kernel (selection function) and the daughter distribution function (breakage function). There are several alternative methodologies for determination of these two functions: (i) experimental, (ii) theoretical, or (iii) computational by detailed mechanistic modelling of the breakage of single particles.

Our previous work [1] we have developed a DEM framework for detailed numerical simulation of needle-shaped crystals movement and breakage. A randomly-packed bed of elongated particles with a given PSD has been formed by letting the particles to settle down by gravity. The bed of particles has been subjected to uni-axial stress by compressing it by two parallel planes. The PSD and all breakage events have been recorded during the compression. In a follow-up work [2], results from these computational (in-silico) experiments were used to identify both the breakage kernel and the daughter distribution functions.
Our current objective is to extend our methodology [1, 2] which has been so far verified for uni-axial compression to more general stress fields.

2 METHODOLOGY

A methodology based on the discrete element method [3] modified to treat non-spherical particles by the multi-element model [4] has been used to simulate the movement and breakage of individual needle-shaped particles. The magnitude and the location of contact forces at each particle determine the load on the particle. Particles are treated as loaded beams in order to calculate bending and shear stresses along the particle. When a set threshold value anywhere along a particle is exceeded the particle breaks into two daughter particles at the point of maximum stress. A full description of the algorithm has been given in our earlier work [1]. Although only normal contact forces among elements of different particles are considered, the particles are not completely frictionless because of theirs geometry. They are represented as a compound of overlaid spherical elements, particle roughness is thus caused by gaps between elements. The set-up of computational experiment is illustrated in Fig 1.

Systems of two sizes have been generated for the simulation of shear induced particle breakage. Smaller systems containing initially 100 particles composed of 20 discrete elements (length = 20) were used for relatively fast simulations aimed to test wide range of model parameters. Selected set of parameter values has then been used in simulations with larger systems of 500, 20-elements long particles. Packing have been generated in the simulation box by letting particles to settle-down on the flat boundary by the gravitation force in the z-axis direction. Periodic boundary condition were imposed in the x- and y-axis directions to avoid the influence of walls. During the next step, another boundary wall has been placed above the simulation box and the packing has been gradually compressed between the two walls. Particles whose loading exceeded a set threshold were allowed to break. In such a way a group of particle systems of different compression ratio has been obtained, cf. Fig 2.

Position of particles near the top and near the bottom of the packing has been frozen.
The lower layer of particles was then forced to move at a specific velocity in the x-th axis direction while the top layer was held still. Particles in between then experience a shearing stress in a similar way as material in the ring shear device. Again, the particles whose loading exceeds a set threshold break into two parts.

3 RESULTS AND DISCUSSION

To find out the effect of the shearing rate on fragmentation of particles in the layer, simulations with different shear rate $v_s$ were carried out. The configuration reached after the layer moved the length 3.15 times the simulation box width is shown in Fig 3. Starting from the same configuration (cf. Fig 2b), lower layer moved at two different speeds. From visual observation it is apparent that more breakage occurred at faster speed (Fig 3a) than at the 50 times slower one (Fig 3b). The breakage takes place mostly in the lower half of the layer in both cases.

Particle size distribution and number mean particle size evolution during shearing is shown in Fig 4. Here the larger and smaller systems are compared. One can see that results for both systems are comparable suggesting that for the computations one can use relatively low number of particles and smaller computational box. Regarding the velocity effect, the fragmentation is lower at slower velocities which is consistent with what one would expect: more careful (slower) particle displacement leaves more time for particle layer rearrangements and thus there is lower chance of local stress built-up and exceeding particle mechanical strength. If the shearing rate is much slower then the rate of layer rearrangements, then the shearing is in a pseudo-steady state and fragmentation does not depend on shearing rate anymore. Even in the pseudo-steady state regime the breakage can still occur if some particles get jammed during their displacement. As we would like to restrict ourselves to situations where the dynamical effects can be neglected, we aim to set the shearing velocity so low to be in the pseudo-steady state regime. It can be seen from results in Fig 4, that the substantial fragmentation occurs at the largest velocity, while there is less fragmentation and lower dependence on shearing velocity at remaining slower velocities.
The simulation is stopped when the shearing distance reaches 6.25 and 12.5 times computation box width in larger and smaller system, respectively. Based on results, this length is sufficient as most of fragmentation occur at the beginning and no more or little fragmentation take place later as all jammed particles broke down and can be freely shifted.

Results investigating the effect of particle strength are introduced in Fig 5. Systems of three different particle strengths at two different compaction ratios are compared. It can be seen that there are small differences between particles of strength 30 and 40 at the lower compaction (88% of the initial particle height). The size of particles further decreases as expected during shearing. It is interesting to observe that the change of size distribution during shearing is smaller for weakest particles (20) than for stronger particles (40). The explanation is that the weakest particles have already broken more during compaction and short particles are less likely to get jammed and break during shearing.

4 CONCLUSIONS

A preliminary study has been made to investigate the possibility to use in-silico experiments to study breakage of needle-shaped particles under shearing stress. Our objective is to use these results in identifying breakage kernels and the daughter distribution functions. We have demonstrated that the simulation of shearing induced breakage is feasible even for modestly sized systems. There are two regimes in respect to the shearing velocity: The breakage depends on shearing velocity at high velocities. However, breakage is velocity independent when the shearing velocity is low enough. More simulations will be necessary to identify the transition between these regimes.
Figure 4: Effect of shearing velocity: Initial and final particle size distribution at different shearing velocities. Number average particle length evolution during shearing. Plots a) and b) are for smaller system, while plots c) and d) are for larger system. Shearing distance is dimensionless, with the unit length corresponding to the diameter of single element. Shearing velocity is also denoted in dimensionless units.
Figure 5: Effect of particle strength: Initial and final particle size distribution with particle strength of 20, 30 and 40 kPa. Number average particle length evolution during shearing. Plots a) and b) are for low compaction ratio (88%). Plots c) and d) are for higher compaction ratio (76%). Shearing distance is dimensionless, with the unit length corresponding to the diameter of single element.
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INCIPIENT SEDIMENT TRANSPORT FOR NON-COHESIVE LANDFORMS BY THE DISCRETE ELEMENT METHOD (DEM)

R. Bravo*, P. Ortiz* and J.L. Pérez–Aparicio†

*University of Granada
Escuela de Caminos
Campus de Fuentenueva, 18071 Granada, Spain
e-mail: rbravo@ugr.es, portiz@ugr.es

†Department of Continuum Mechanics and Theory of Structures
Universidad Politécnica de Valencia
Camino de Vera s/n. 46022. Valencia, Spain
e-mail: jopeap@upvnet.upv.es

Key words: Granular Materials, DEM, FEM, Contact Problems

Abstract. The determination of the shear stress at which a sediment grain of a given size and density starts to move has been treated with theoretical, experimental and numerical procedures by many authors. The seminal contribution of Shields [7] addresses a relationship for the non-dimensional critical shear stress in terms of the friction Reynolds number for a single particle in a flat bed.

This work focusses on the incipient transport of particles for bedforms. The proposed numerical approach to the problem integrates the Discrete Element Method (DEM) [9] with a continuous finite element approximation. The DEM simulates the motion of the landform, defined as an aggregate of rigid discs that interact by contact and friction. The continuous finite element approach predicts the boundary shear stress field coming from the fluid flow over the bed (for basic formulation, see [4] and reference therein). Both methods are coupled through the flow-particle force transmission using drag coefficients. While for single particles (or very simple sets of particles) incipient motion (and consequently, the threshold stress) is clearly defined, for complex forms the use of the concept of incipient transport becomes necessary, and critical shear stress is established in terms of a threshold sediment flux over the bed surface.

We present a series of numerical experiments for single particles, showing good agreement with Shields curve for the whole range of Reynolds number. In this communication we show some of these results, in compare with the basic Shields curves for flat bed and single grains.
1 Introduction

The mechanics of sediment transport is the keystone of many fields. Many authors have carried out experimental studies to analyze, measure and predict the sediment transport under many conditions since there is not a general analytical formulation or a numerical approach that analyzes the sediment transport accurately. This paper establishes a new numerical approach in the analysis of the motion treshold of granular particles, simulating the initiation of sediment transport in the interface between fluid and sediment through the numerical coupling of the Discrete Element Method (DEM) for particles and the Finite Element Method for fluid.

Shields was the first reference to define a curve that defines the initiation of motion relating and the Reynold’s number. This curve was based in dimensional considerations and experimental data, therefore it was not able to define the motion of the individual particles. The new approach considers the real behaviour of granular materials simulating the entrainment kinematics and particle interactions through contact. The Discrete Element Method is a powerful tool to model the geometry and interactions since its formulation is based in the balance momentum equation plus the additional restrictions with contact. The flow interaction is inserted in model using the lift and drag forces from [3]. The proposed work obtains the initiation of motion for situations in which shield’s curve is not able to provide reliable data.

2 Analytical theory

The available analytical theories [3], [8] are based in the analysis of the motion of a single particle over a sediment bed. This situation is depicted in Fig. 1 where the motion of the underneath particles is restricted, therefore it represents the worst situation. If the scheme from Fig. 1 is repeated periodically, then it represents a sediment bed Fig. 2.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Single particle over a sedimentary bed}
\end{figure}

The balance of forces of Fig. 1 allows to obtain the combination of drag $F_d$ and lift $F_l$ forces for any friction angle $\phi$ and compacity angle $\theta$ that initiates the motion of a single
Figure 2: Sedimentary bed, obtained as a periodic repetition of the scheme depicted in Fig. 1

particle. Solving these equations it is possible to obtain the normal \( N \), tangential forces \( T \) and the relation between \( F_d \) and \( F_l \) for the initiation of motion.

\[
F_l + F_d \tan \theta = W; \quad T = F_d \sin \theta + (F_l - W) \cos \theta; \\
N = F_d \tan \theta(1 - \sin \theta) + (W - F_l) \sin \theta
\]  

This equilibrium equation allows to obtain the relation between \( u^* \) and the Reynolds number \( R^* \) that forces the for two situations

2.1 Small Reynolds Numbers

In this section we briefly describe the derivation of the drag for drag \( F_d \) and lift forces \( F_l \) as function of shear frictional velocity \( u^* \) and therefore a relationship between shear stress \( \tau = u^{*2} \rho_f \) and Reynolds number \( Re^* \) for a single particle of diameter \( d \). These expressions inserted in Eqs. 1 provide the condition for the initiation of motion as function of \( u^* \). For low Reynolds number \( R^* < 30 \), the velocity distribution around the particle is linear. Therefore the mean flow velocity is defined as:

\[
V_f = \frac{u^*^2}{2 \nu} d; \quad \text{while } F_d \text{ and } F_l \text{ are given by: } F_d = \frac{3}{2} \pi \tau d^2; \quad F_l = \frac{1}{2} \frac{u^*^2 d}{\nu} \tau d^2
\]  

where \( \nu \) is the viscosity, \( \rho_s \) and \( \rho_f \) are the densities of the solid and fluid respectively. Combining Eqs. 1 and 2 provides a relation between \( u^* \) and the Reynolds number:

\[
\frac{\tau}{(\rho_s - \rho_f)gd} = \frac{\pi/6}{3\pi \tan \theta + \frac{1}{2} \frac{u^*^2}{\nu}}
\]  

2.2 Large Reynolds Numbers

For large Reynolds number \( R^* \geq 30 \) the velocity distribution around the particle is logarithmic and is given by the following expression:

\[
\frac{u}{u^*} = 2.5 \log \frac{z}{z_0} \quad \frac{\partial u}{\partial z} = 2.5 u^* \frac{1}{z}
\]  

Using these last two results the expressions for the drag \( F_d \) and lift \( F_l \) forces are:
\begin{equation}
F_d = \frac{1}{8} C_d \pi \frac{V_f^2}{u^*} \tau d^2; \quad F_l = \frac{V_f}{u^*} \left( \frac{\partial u}{\partial z} \right) \left( \frac{u^* d}{\nu} \right) \left( \frac{u^* d}{\nu} \right)^{0.5} \tau d^2; \quad (5)
\end{equation}

In similar way as in the previous subsection, it is possible to define an adimensional relation that provides \( u^* \) as function of \( R^* \).

\begin{equation}
\frac{\tau}{(\rho_s - \rho_f)g d} = \frac{\pi/6}{\nu} \left( \frac{24 \nu}{d} \right)^{0.5} \left( \frac{u^* d}{\nu} \right)^{0.5} + \frac{\pi}{8} C_d \left( \frac{V_f}{\nu} \right)^2 \quad (6)
\end{equation}

3 DDA GENERIC FORMULATION

3.1 Introduction

From the pioneering work of [6] on the Discrete Element Method (DEM), [5] extended this method to another one called Discrete Deformation Analysis (DDA) for the analysis and modeling of the mechanical response of rock assemblies. The reason for DDA’s reliability is that it reflects the mechanics of the phenomenon associated with the movement of the particles; beyond the exact representation of basic material and geometrical properties, it simulates mechanical interactions explicitly.

3.2 Governing equations

This subsection describes the problem and the corresponding governing equations including the contact equation in DDA based on Hamiltonian mechanics.

3.2.1 Hamiltonian description of motion

Hamiltonian mechanics permit to obtain the equations of motion for every point of multiple particles that interact by contact. The particles are still considered a continuum. Each point \( x, y \) in each particle \( i \) is characterized by its position \( Q^i(x, y, t) \) and its linear momentum \( P^i(x, y, t) \). The Hamiltonian function \( H \left[ Q(x, y, t), P(x, y, t) \right] \) defines the total energy of the set of particles, that is assumed to be separable in kinetic \( K(P(x, y, t)) \) and potential \( \Pi(Q(x, y, t)) \) energies:

\begin{equation}
H \left[ Q(x, y, t), P(x, y, t) \right] = \sum_{i=1}^{n_{pd}} \left[ K(P^i(x, y, t)) + \Pi(Q^i(x, y, t)) \right]
\end{equation}

\begin{equation}
K(P^i(x, y, t)) = \frac{1}{2} \int_{\Omega^i} \frac{P^i(x, y, t)^2}{\rho_s} d\Omega; \Pi(Q^i(x, y, t)) = \int_{\Omega^i} Q^i(x, y, t)^T f(Q^i(x, y, t)) d\Omega
\end{equation}
where \( n_{bd} \) is the total number of particles and \( \Omega^i \) the particle domain. The kinetic and potential energies are real scalar functions and \( \rho_s \) is the particle density, assumed constant. In this work, the potential energy \( \Pi \) is related with forces external and due to contact, generically represented in Eq. 7 by \( f(Q^i(x, y, t)) \). The motion of particle \( i \) is then governed by the Hamiltonian canonical equations [2]:

\[
\begin{align*}
\dot{Q}^i(x, y, t) &= \frac{\partial H(Q(x, y, t), P(x, y, t))}{\partial P^i} = \int_{\Omega^i} \frac{P^i(x, y, t)}{\rho_s} \, d\Omega \\
\dot{P}^i(x, y, t) &= -\frac{\partial H(Q(x, y, t), P(x, y, t))}{\partial Q^i} = -\nabla \Pi(Q^i(x, y, t))
\end{align*}
\]

and where the supra dot indicates derivative with respect to time.

### 3.2.2 Discretization

Often it is not possible to find an analytical solution of the previous equations; we have to obtain an approximated solution through the discretization of variables \( Q, P \) from Eqs. 8. For every point \( x, y \) of particle \( i \), these variables are interpolated from values defined at several points called nodes.

\[
Q^i(x, y, t) = N(x, y) \, q^i(t) ; \quad P^i(x, y, t) = N(x, y) \, p^i(t)
\]

where \( N \) is the shape function associated to the node, usually defined at the center of gravity \( x^i, y^i \). These shape function matrix contain the interpolating polynomials, see an example in subsection 5. Usually in DDA a single node is defined at the gravity center and consequently the variables at this node are the unknowns of the problem. These nodal displacements \( q^i \) and linear momenta \( p^i \) for all particles nodes at a given time are grouped in the vectors \( q(t), p(t) \).

For each particle \( i \), the discretization Eqs. 9 combined with Eqs. 8 produce the system of equations:

\[
\begin{align*}
\dot{q}^i &= M^{-1}_i \, \dot{p}^i ; \quad \quad \dot{p}^i = -N^T \nabla \Pi(Nq^i) = f_c^\nu + f_{ext}^\nu
\end{align*}
\]

where \( M^{-1}_i \) is the inverse of a diagonal mass matrix, with entries \( M_i = \int_{\Omega^i} N^T \rho_s \, N \, d\Omega \) and \( \dot{p} \equiv f_c^\nu + f_{ext}^\nu \) is the discrete counterpart for Newton’s second law (contact forces \( f_c^\nu \) plus the discrete external \( f_{ext}^\nu \)). Finally, Eqs. 10 are integrated in time using the energy consistent formulation of [1].
4 DESCRIPTION OF CONTACT

Consider two rigid particles \(i, k\) the domains of which are defined by \(\Omega^i, \Omega^k\) and with boundaries \(\Gamma^i = \partial \Omega^i, \Gamma^k = \partial \Omega^k\) (Fig. 3). These particles interact through contact and it is possible to obtain the magnitude that defines the separation between particles by the gap function:

\[
g_{ik}^N(X) \leftrightarrow g_{ki}^N(Y(X)) = q^i(X) - q^k(Y(X)) \quad R_{ki}^{11}
\]

The variables \(q^i(X)\) and \(q^k(Y(X))\) are the positions of the closest-points \(X, Y\) and \(R_{ki}\), see Fig. 3, is the normal unit vector. The gap function has to satisfy the constraint \(g_{ik}^N \geq 0\) or impenetrability condition.

![Figure 3: Contact between two particles \(i, k\): closest point projection mapping](image)

5 Numerical coupling

We are going to focus on the coupling of \(F_d\) and \(F_l\) in DEM considering like point forces applied in the center of gravity of each mass. Without loss of generality we consider a
point force $F_x, F_y$ applied in $(x, y)$ and subjected to $(Q_x, Q_y)$. Therefore the potential energy is:

$$\Pi_i = -(Q_x F_x + Q_y F_y) = -\begin{pmatrix} Q_x \\ Q_y \end{pmatrix}^t \begin{pmatrix} F_x \\ F_y \end{pmatrix} = -q_i^t \begin{pmatrix} N^t_i \begin{pmatrix} F_x \\ F_y \end{pmatrix} \end{pmatrix}$$

(13)

Minimizing $\Pi_i$ respect to $q_i^t$:

$$\frac{\partial \Pi_i}{\partial q_i^t} = \frac{\partial}{\partial q_i^t} q_i^t \begin{pmatrix} N_i(x, y)^t \begin{pmatrix} F_x \\ F_y \end{pmatrix} \end{pmatrix} = N_i^t \begin{pmatrix} F_x \\ F_y \end{pmatrix} \rightarrow f_{ext}$$

(14)

Therefore, substituting the $x, y$ components of the discrete point drag and lift forces in $F_x, F_y$ given by the NStokes formulation in every time step and applying in gravitus center of each body, we obtain the expression for these forces in DEM.

6 Description of the coupled numerical model

6.1 Description of NStokes

Accurate prediction of sediment transport depends on a proper computation of stresses in the boundary layer. The computed stress field is obtained from the flow by means of a continuous finite element model for the incompressible Navier-Stokes equations (for details see Refs. [10] and [4]). Once stress field is calculated, values on the boundary layer are used to compute drag and lift forces by transforming shear stresses to drag and lift forces using Eqs. 2.

7 Numerical results

7.1 Shields diagram for flat surface

Analytical formulation for the initiation of sediment motion is usually based on the following dimensionless relation:

$$\frac{\tau}{(\rho_s - \rho_f) g d} = F \left( \frac{u^* d}{\nu} \right).$$

The famous Shields diagram [7]
was obtained fitting the previous relation to the experimental data and is depicted in Fig. 7.1.3. The numerical approach simulates accurately the micromechanics that analytical formulations cannot take into account, like the rolling or sliding between particles for several geometries and frictional materials. In order to prove the efficiency of the numerical approach, this will be applied to simulate the analytical formulation from [3] and the experimental data from Shields.

7.1.1 Numerical setup

The experimental setup is depicted in Fig. 1, where the rigid lateral boundaries avoid the motion of spheres 1 and 2 while sphere 3 may slide or roll over them. This configuration is computationally attractive since it simulates a periodic boundary, see Fig. 2 that prevents the displacement of spheres 1 and 2. These particles do not roll due to the high imposed friction coefficient.

In this situation, only particle 3 interacts with fluid since it is considered that the motion is parallel to the surface. It is expected that the numerical approach fits well the analytical ones due to both have the same set up. In this simple case, sphere 3 is only affected by the fluid force using drag and lift forces \( F_d \) and \( F_l \) defined by coefficients \( C_d \) and \( C_l \).

7.1.2 Solution procedure.

As seen in Shields diagram [7] and analytical formulations [3], several variables depend both the \( x \) and \( y \) axes, therefore we have to use an iterative procedure to obtain the solution that represents the initiation of motion. This is summarized in these steps:

- Input data: initial \( d \), final \( d \), increment of \( \Delta d \), \( \Delta u^* \), \( \nu \), tol.
- For every size \( d \):
  - Start wit a given \( u^* = \Delta u^* \)
  - Compute \( Re^* \), the decide if laminar or turbulent situation is reached. Usually laminar for \( Re^* < 5 \).
  - Compute drag and lift forces \( f_d \), \( f_l \) and apply to sphere.
  - Verify initiation of motion with DDA.
    - If total displacement < tol. No motion, then \( u^* = u^* + \Delta u^* \) and go to the second item.
    - Otherwise. Compute \( \tau^* \). \( d = d + \Delta d \)

After applying this procedure, the diagram depicted in Fig. 7.1.3 is obtained. It is important to remark that for \( 5 < Re^* < 30 \) there is a transition from laminar to turbulent flow that makes difficult that the numerical and analytical data fit wit the experimental ones.
7.1.3 Analysis results

Fig. 7.1.3 shows the numerical, analytical and experimental results for the Shields diagram. Analytical results show two limiting situations, that correspond to the initiation of motion by rolling or lifting. The experimental and numerical results fall between this situations. It is clear that the numerical model only predicts the initiation of motion by rolling since the numerical model is only able to simulate such initiation. For low $Re^*$ the drag force $F_d$ is linear, then the left part of the logarithmic Shield’s diagram is almost planar. Real particles are not fully spherical, then the drag coefficient $C_d$ and the friction is higher than that for a sphere and a high stress $\tau^*$ is needed to initiate the motion. That is the reason that experimental results provides higher values than the analytical and experimental. For turbulence, the velocity distribution around particles is logarithmic, therefore the relation given by the right part of the logarithmic graph is linear.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{Shields diagram for a single particle, experimental, analytical and numerical results}
\end{figure}

7.2 Shields diagram for inclined surfaces

This example analyses the initiation motion of the external inclined sides of a triangular shaped assembly composed by thousands of circular rigid particles of the same radius, as shown in Figs. 7.2.2. This analysis is focused in the surface particles since this is the interface between landform and fluid.

7.2.1 Set up

The internal geometry of the landform is defined by disks of the same radius disposed with an arrangement that provides the maximum packaging. The geometry of the shape
is defined by the following parameters: inclination of the sides \( \alpha \) and height \( h \). The disks are geometrically defined by its radii and the mechanical parameters: density \( \rho_s \), friction coefficient \( \mu \) (or friction angle \( \phi \)). No cohesion is considered. Radii, the friction and inclination angles define the global stability of the landform. In order to reach stability, the friction angle \( \phi \) has been chosen to be greater than the inclination \( \alpha \).

### 7.2.2 Results

Following the same procedure explained in the previous simulation the numerical relationship \( Re^* - \tau^* \) that forces the general motion of the particles is obtained. According to several papers the initiation of motion is reached when the particles fluid is greater than a given quantity, see [8], that is equal to an equivalent number of particles dependent of the particle radius. This relationship shown in Figs. 7.2.2 for several inclinations \( \alpha \), showing a similar relationship to Shields diagram. The results are higher than the previous since the inclination \( \alpha \) makes difficult the motion of the particles upwards due to the inclined component of the weight. Additionally, the numerical results show that \( \tau^* \) are always greater than the experimental since the latter are measured over a flat surface. \( \tau^* \) grows with \( \alpha \) since as \( \phi \) increases it is more difficult to move the particle upstream. Inclination \( \alpha \) must be always lower than \( \phi \) to prevent the collapse of the assembly. For larger radii particles, the numerical data highly differ from Shields since the geometry of the sides is quite rough that makes the motion difficult. This phenomenon is increased with \( \alpha \).

![Figure 6: \( Re^* - \tau^* \) relationship for multiple inclinations \( \alpha \). Comparison with experimental data for flat bed from Shields](image-url)

The rolling upwards is usual mechanism for the initiation of motion. Particles never roll downwards since the friction and drag forces avoid that kind of motion. The motion
usually starts on the top side of the landform since in this location the gradient of the flow velocities is high and the motion of the particles is not so restricted. Due to the high gradient on the top particles usually lift, while those situated on the bottom and middle roll, as shown in the three snapshot depicted in Figs. 7.2.2 where it is clear that the initiation of motion always starts in the upstream side and particles climb over the existing ones.

![Figure 7: Snapshots at several instants in which the initiation of motion is produced](image)

8 CONCLUSIONS

- A coupled numerical model has been applied to simulate the initiation of motion of landforms combining DEM-FEM.

- The Discrete Element Method allows to simulate the micromechanics of the landform, therefore it provides realistic results that fit well to the experimental given by Shields. Additionally, FEM gives a good representation of the flow that acts over the landform.

- The coupled numerical method has been able to simulate accurately the experimental results and that for no experimental are available. Therefore it converts in a powerful tool to simulate the initiation of motion in complex situations where analytical results are not valid.

- It is expected to model accurately more complex problems increasing the number of particles although the parallelization will be needed.
REFERENCES


SIMULATION OF SOLUTE TRANSPORT IN 3D POROUS MEDIA USING RANDOM WALK PARTICLE TRACKING METHOD

YUANYUAN SUN\textsuperscript{1,3*}, CHAN-HEE PARK\textsuperscript{2}, WENQING WANG\textsuperscript{1} AND OLAF KOLDITZ\textsuperscript{1,3}

\textsuperscript{1}Helmholtz Centre for Environmental Research (UFZ)
Department of Environmental Informatics
Permoserstrasse 15, 04318 Leipzig, Germany
e-mail: yuanyuan.sun@ufz.de, olaf.kolditz@ufz.de, www.ufz.de/

\textsuperscript{2}Korea Institute of Geoscience and Mineral Resources (KIGAM)
Geothermal Resources Department
92 Gwahang-no, Yuseong-gu, Daejeon 305-350, Korea
e-mail: chanhee.park@kigam.re.kr, www.kigam.re.kr/

\textsuperscript{3}TU Dresden
Applied Environmental System Analysis
Helmholtzstrasse 10, 01062 Dresden, Germany

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Abstract. Random walk particle tracking (RWPT) method provides a computationally effective way to characterize solute transport process in porous media. In this work, an object-oriented scientific software platform OpenGeoSys (OGS) was adopted for the simulation and visualization of the complex behavior of particles. Finite element method is used for the calculation of the velocity field which is necessary for the determination of the displacement of the particles through space.

The RWPT method has been used in the simulation of the hydraulic process, diffusion and dispersion as it is proved to be well suited for such studies. In this work, efforts were taken to search for the solution to simulate the retardation and decay processes in order to investigate the effects that appear in the contaminant plume evolution. Expressions for the effective coefficients governing the solute transport are derived for retardation model, based on a two-rate sorption-desorption approach.

The RWPT model was first verified by a benchmark test of solute transport in a one-dimensional homogeneous media to analyse the accuracy of the method with comparison to the analytical solution. The analysis was then extended to applications with three-dimensional homogeneous aquifer. This method can be used as a tool to elicit and discern the detailed structure of evolving contaminant plumes.
1 INTRODUCTION

Eulerian and Lagrangian transport models are two basic approaches in numerical simulation of solute transport. The first one has limitations in application of numerical dispersion, thus a higher grid resolution and smaller time steps have to be applied\(^1\). Whereas the latter avoids solving the transport equation directly, therefore does not need such consideration, the computational times are reduced. But the Lagrangian approach also has disadvantage when applied to dissipative systems. RWPT method was developed basing on the Lagrangian concept. A finite number of particles represent the distribution of the solute mass in porous media and their behavior can be observed\(^2\). The particles are moved through the porous media according to the velocity field obtained from the solution of the flow equation.

RWPT method has been used for modeling solute transport in aquifers\(^3\), complex, high-resolution transport problems\(^4, 5\), advective-dispersive transport in composite media\(^6\), fractional-order multiscaling anomalous diffusion\(^7\), non-Fickian transport\(^8\).

There are other concepts of particle tracking methods, for instance, continuous time random walk (CTRW)\(^9, 10, 11\), and convolution-based particle tracking (CBPT)\(^12\). Particle tracking methods have been frequently adopted in the study of flow and solute transport in groundwater modeling. The most common applications are for the delineation of path lines in a flow model. Softwares have the module of particle tracking (MODFLOW), or provide a visualization tool for the path lines and travel times simulation (FEFLOW, ParaView). Most of the researches using particle tracking method only considered the advective-dispersive process, few of them mentioned about retardation and decay. To this purpose, a RWPT model was established on an scientific software platform OpenGeoSys (OGS)\(^13, 14\) as discussed in the following section.

The OGS project is an open source initiative for numerical simulation of thermo-hydro-mechanical-chemical (THMC) processes in porous media. Finite element method was used for the calculation of the velocity field. In the RWPT simulation, a finite number of particles were injected into the calculation domain\(^15\), the mobility of the particles was controlled by using retardation and decay models. The number of particles that leave the domain was counted to produce the breakthrough curves.

2 THEORY

This work made use of the groundwater flow model implemented in OGS\(^13, 14\). The model deals with saturated subsurface flow. The governing equation for groundwater flow is the fluid mass balance equation. Darcy’s law is used for momentum balance.

2.1 Transport Model

The classical advection-dispersion equation of a conservative solute in porous media can be written as\(^16\)

\[
\frac{\partial C}{\partial t} = -\nabla \cdot (v C) + \nabla \cdot (D \nabla C)
\] (1)
where $C$ is the mass concentration $(ML^{-3})$, $\mathbf{v}$ is the pore velocity vector $(ML^{-1})$, and $D$ is the hydrodynamic dispersion tensor $(L^2T^{-1})$, $t$ is time $(T^2)$ and $\nabla$ is the differential nabla operator.

2.2 The Random Walk Particle Tracking (RWPT) Method

The RWPT method is issued from stochastic physics. The stochastic differential equation is

$$x(t_i) = x(t_{i-1}) + \mathbf{v}(x(t_{i-1}))\Delta t + Z\sqrt{2D(x(t_{i-1}))\Delta t}$$

(2)

where $x$ is the coordinates of the particle location, $\Delta t$ is the time step, and $Z$ is a random number whose mean is zero and variance is unit.

It has been shown that this equation is equivalent to an expression that is slightly different from the advection-dispersion equation (1). To be equivalent to equation (1), the modified velocity is expressed as

$$v_i^* = v_i + \sum_{j=1}^{3} \frac{\partial D_{ij}}{\partial x_j}$$

(3)

with dispersion tensor

$$D_{ij} = \alpha_T|\mathbf{v}|\delta_{ij} + (\alpha_L - \alpha_T)\frac{v_jv_i}{|\mathbf{v}|} + D_{ii}^d$$

(4)

where $\delta_{ij}$ is the Kronecker symbol, $\alpha_L$ is the longitudinal dispersion length, $\alpha_T$ is the transverse dispersivity, $D_{ii}^d$ is the tensor of molecular diffusion coefficient, and $v_i$ is the component of the mean pore velocity in the $i$th direction.

The equivalent stochastic differential equation to (1) in three dimensional problems can be written as

$$x_{t+\Delta t} = x_t + \left(v_x(x_t,y_t,z_t,t) + \frac{\partial D_{xx}}{\partial x} + \frac{\partial D_{yx}}{\partial y} + \frac{\partial D_{zx}}{\partial z} \right)\Delta t + \sqrt{2D_{xx}\Delta t}Z_x$$

(5)

$$y_{t+\Delta t} = y_t + \left(v_y(x_t,y_t,z_t,t) + \frac{\partial D_{yy}}{\partial x} + \frac{\partial D_{yx}}{\partial y} + \frac{\partial D_{zy}}{\partial z} \right)\Delta t + \sqrt{2D_{yy}\Delta t}Z_y$$

$$z_{t+\Delta t} = z_t + \left(v_z(x_t,y_t,z_t,t) + \frac{\partial D_{zz}}{\partial x} + \frac{\partial D_{zr}}{\partial y} + \frac{\partial D_{zz}}{\partial z} \right)\Delta t + \sqrt{2D_{zz}\Delta t}Z_z$$

where $Z_i$ is the corresponding directional random number.

Together with equation (4), the spatial derivatives of the dispersion coefficients can be expressed as a function of the derivatives of velocity. Note that to obtain the derivatives of velocity, velocity has to be continuous function. For this end, we interpolate velocity at any location in an element from the known velocity at the element nodes.
Since the proposed RWPT method makes use of the FEM for velocity estimation, the derivative of velocity within each element is computed as in Fig. 1 and written as

\[
\frac{\partial v_x}{\partial x} = \frac{v(x_L) - v(x_R)}{l_x}, \quad \frac{\partial v_y}{\partial y} = \frac{v(y_D) - v(y_U)}{l_y}, \quad \frac{\partial v_z}{\partial z} = \frac{v(z_N) - v(z_S)}{l_z}
\]

where \(x_L\) and \(x_R\) are the intersectional points of the element edges with an extension of a line parallel to the global \(x\) axis at which velocities are \(v(x_L)\) and \(v(x_R)\), \(y_D\) and \(y_U\) are the intersectional points of the element edge from down to up with extension of the line parallel to the global \(y\) axis at which velocities are \(v(y_D)\) and \(v(y_U)\), \(z_S\) and \(z_N\) are the intersectional points of the element edge from south to north with extension of the line parallel to the global \(z\) axis at which velocities are \(v(z_S)\) and \(v(z_N)\), and \(l_x\), \(l_y\), and \(l_z\) are the length of each intersectional line respectively.

Figure 1: Spatial derivatives of velocity for a particle in triangular and quadrilateral elements

Thus, the derivatives of the dispersion coefficients are as follows: \(^{(21)}\)

\[
\begin{align*}
\frac{\partial D_{xx}}{\partial x} &= v_x \frac{\partial v_x}{\partial x} \left[ \alpha_L \left( \frac{2}{v^3} - \frac{v^2}{v^3} \right) - \alpha_T \frac{v^2 + v^4}{v^5} \right] \\
\frac{\partial D_{xy}}{\partial y} &= \left( \alpha_L - \alpha_T \right) \frac{\partial v_y}{\partial y} v_x v_y \left( \frac{1}{v^3} + \frac{v}{v^4} \right) \\
\frac{\partial D_{xz}}{\partial z} &= \left( \alpha_L - \alpha_T \right) \frac{\partial v_z}{\partial z} v_x v_z \left( \frac{1}{v^3} + \frac{v}{v^4} \right) \\
\frac{\partial D_{yy}}{\partial y} &= v_y \frac{\partial v_y}{\partial y} \left[ \alpha_L \left( \frac{2}{v^3} - \frac{v^2}{v^3} \right) - \alpha_T \frac{v^2 + v^4}{v^5} \right] \\
\frac{\partial D_{yz}}{\partial z} &= \left( \alpha_L - \alpha_T \right) \frac{\partial v_z}{\partial z} v_y v_z \left( \frac{1}{v^3} + \frac{v}{v^4} \right) \\
\frac{\partial D_{zz}}{\partial z} &= \left( \alpha_L - \alpha_T \right) \frac{\partial v_z}{\partial z} v_z^2 \left( \frac{1}{v^3} + \frac{v}{v^4} \right)
\end{align*}
\]
Because velocity is not derivable at the interface of two adjacent element in a nonuniform flow, computing dispersion coefficient derivatives by using a finite element approach would yield erroneous values\(^{[21]}\). To prevent the errors, a particle is coded to have information of an element index and the velocity estimation is continuous even at the elemental boundaries in this method. Thus, the derivatives of dispersion coefficients will be computed accordingly. This is an improved approach from the work by\(^{[21]}\).

3 TRANSPORT IN ONE-DIMENSIONAL SOIL COLUMN

A one-dimensional homogenous aquifer is chosen to simulate a soil column experiment conducted by Harter et al.\(^{[22]}\). In the experiment, a constant flow rate was established, 2.5 pore volumes NaCl - tap water solution and 2.5 pore volumes Cryptosporidium parvum solution \((1 \times 10^5\) oocysts per mL\) were injected respectively, the outflow was continuously collected. Fig. 2 shows the schematic description of the experiment.

NaCl - tap water solution is used as tracer, which experiences only advection and dispersion. The Cryptosporidium parvum can be classified as biological colloid. Colloids moving in porous media experience advection, dispersion, sorption-desorption, and filtration.

3.1 Analytical Solution

For one-dimensional transport including sorption-desorption and filtration through a homogeneous medium the following differential equation is applied

\[
\frac{\partial C}{\partial t} + \frac{\rho_b}{n} \frac{\partial C_S}{\partial t} = v \alpha_L \frac{\partial^2 C}{\partial x^2} - v \left( \frac{\partial C}{\partial x} + \lambda C \right)
\]

where \(C\) is dissolved concentration (kg·m\(^{-3}\)), \(C_S\) is sorbed concentration(kg·kg\(^{-1}\)), \(t\) is time (s), \(\rho_b\) is bulk density (kg·m\(^{-3}\)), \(n\) is porosity (-), \(v\) is velocity (m·s\(^{-1}\)), \(\alpha_L\) is longitudinal
dispertivity (m), $x$ is distance (m), $\lambda$ is filtration coefficient (m$^{-1}$). The instantaneous, linear sorption model assumes that

$$C_S = K_d C$$

(9)

where $K_d$ is the partitioning coefficient (m$^3$ · kg$^{-1}$). The retardation coefficient $R$ is

$$R = 1 + \frac{\rho b}{\theta} K_d$$

(10)

The dispersion coefficient in $x$-direction $D_{xx}$ (m$^2$ · s$^{-1}$) is

$$D_{xx} = v \alpha L$$

(11)

The analytical solution for a pulse input (inject time from 0 to $\tau$) is

$$C = \frac{1}{2} C_0 \left[ \exp \left( \frac{vx(1 - \gamma)}{2D_{xx}} \right) \text{erfc} \left( \frac{x - v\gamma t/R}{2\sqrt{D_{xx}t/R}} \right) + \exp \left( \frac{vx(1 + \gamma)}{2D_{xx}} \right) \text{erfc} \left( \frac{x + v\gamma t/R}{2\sqrt{D_{xx}t/R}} \right) \right]$$

(12)

for $t \in (0, \tau)$, where

$$\gamma = \sqrt{1 + 4v\lambda RD_{xx}/v^2}$$

(14)

$$\gamma = \sqrt{1 + 4v\lambda RD_{xx}/v^2}$$

(14)

3.2 Numerical Solution

The calculation area is simplified to a line with the length of 0.1m. For the numerical model 100 elements and 101 nodes are included. Head gradient is set by giving two constant pressures at both left and right boundaries to establish a uniform velocity field with the value of 7.1 md$^{-1}$. 
The number of pore volume (x-axis) is calculated by

\[ P_V = \frac{vt}{L} \]  

(15)

where \( v \) is the seepage velocity, \( L \) is the length of the soil column. The time step size is set by assigning \( P_V \) to 0.01. In the simulation, 100 particles per time steps are loaded near the left boundary for 250 time steps.

The filtration process is described by using the filtration coefficient. The sorption-desorption process is described by the two-rate model from Johnson et al.[23]. In the two-rate model, desorption is governed by two different rate coefficients

\[ \frac{N}{N_0} = Ae^{-k_1t} + (1 - A)e^{-k_2t} \]  

(16)

where \( N \) is the number of particles remaining on the medium at time \( t \), \( N_0 \) is the initial number of particles on the medium at the time of initial sorption, \( A \) is a weighting factor, \( k_1 \) and \( k_2 \) are the fast and slow sorption rate coefficient, respectively. Relative parameters are listed in Tab. 1.

Table 1: Model parameters for the column experiment

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k )</td>
<td>Permeability</td>
<td>1.114476 (^{-11})</td>
<td>m(^2)</td>
</tr>
<tr>
<td>( \alpha_{L} )</td>
<td>Longitudinal dispersion length</td>
<td>0.005</td>
<td>m</td>
</tr>
<tr>
<td>( n )</td>
<td>Porosity(tracer)</td>
<td>0.5</td>
<td>–</td>
</tr>
<tr>
<td>( n )</td>
<td>Porosity(colloid)</td>
<td>0.42</td>
<td>–</td>
</tr>
<tr>
<td>( A )</td>
<td>Weighting factor</td>
<td>0.9</td>
<td>–</td>
</tr>
<tr>
<td>( k_1 )</td>
<td>Fast sorption rate coefficient</td>
<td>0.1</td>
<td>–</td>
</tr>
<tr>
<td>( k_2 )</td>
<td>Slow sorption rate coefficient</td>
<td>0.001</td>
<td>–</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>Filtration coefficient</td>
<td>5.2</td>
<td>( m^{-1})</td>
</tr>
</tbody>
</table>

### 3.3 Results

The tracer experiences only advection and dispersion, which means in Equation (8), \( C_S = 0 \), \( \lambda = 0 \). The results of RWPT simulation for the distribution of concentration over time are compared to those of measured value from the experiment by Harter[22], the analytical solution, and the OGS simulation with mass transport method. The comparison results are shown in Fig. 3a. The curves fit very well, which indicates the accuracy of this method.

In the colloid transport simulation, the number of particles leaving the right boundary was counted each time step. The number was then converted to concentration in order to obtain the corresponding breakthrough curve over time. The comparison with the measured value from
the experiment by Harter are shown in Fig. 3b. There are five sections in the breakthrough curve, namely the point at which solute is observed, breakthrough, steady state plateau, elution portion, and a persistent tailing. The RWPT method successfully simulated both portions of the curve. The result shows that the method is capable for producing accurate concentrations.

![Image](image-url)

(a) Advection and dispersion  
(b) Sorption-desorption and decay

Figure 3: Colloid transport in a soil column

4 TRANSPORT IN THREE-DIMENSIONAL CUBE

A three-dimensional homogeneous cube is chosen to verify advective dispersive transport. The side length of the cube model domain is 100 m. The velocity field is held constant in the diagonal direction from bottom left to top right (Fig. 4a).

![Image](image-url)

(a) Cube schematic  
(b) Particle clouds

Figure 4: Particle tracking with advection and dispersion in a cube

4.1 Analytical Solution

The stated problem can be compared with an analytical solution provided by\(^{24}\).
\[ C(x, y, z, t) = \frac{C_0V}{8(\pi t)^{3/2}} \frac{1}{\sqrt{D_{xx}D_{yy}D_{zz}}} \exp \left[ -\frac{(x - x_0)^2}{4D_{xx}t} - \frac{(y - y_0)^2}{4D_{yy}t} - \frac{(z - z_0)^2}{4D_{zz}t} \right] \] (17)

where \( C_0 \) is the initial concentration.

### 4.2 Numerical Solution

The domain is discretized with tetrahedral elements. The same grid density is used for converting particle distributions to element concentrations. The head gradient is set by assigning two constant boundary conditions on the diagonal joint points.

The initial source load is applied to an area close to the bottom left of the domain to have an initial concentration of \( C_0 = 1 \text{ kgm}^{-3} \). The material properties for this model setup are given in Tab. 2.

**Table 2: Material properties**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k )</td>
<td>Permeability</td>
<td>6.0804\times10^{-10}</td>
<td>m$^2$</td>
</tr>
<tr>
<td>( \alpha_L )</td>
<td>Longitudinal dispersion length</td>
<td>0.005</td>
<td>m</td>
</tr>
<tr>
<td>( \alpha_T )</td>
<td>Transverse dispersivity</td>
<td>0.005</td>
<td>m</td>
</tr>
<tr>
<td>( n )</td>
<td>Porosity</td>
<td>0.2</td>
<td>–</td>
</tr>
</tbody>
</table>

### 4.3 Results

The advection-dispersion of the particles pulse across the cube is shown in Fig. 4b. The number of particles used for this simulation is 500. Boundary control was applied in the simulation that when a particle reached the surface of the cube, it would be attached. When particles reached the top right point, the number was counted to generate the breakthrough curves.

The result of RWPT simulation for the distribution of concentration over time is compared to the analytical solution. The simulations with various numbers of particles are depicted in Fig. 5. We found that 500 particles are sufficient in this case to fit both maximum and breakthrough time, which saves computation time. Computation time is linear relative with the number of particles according to the simulation we applied.

### 5 CONCLUSIONS

In this work, RWPT model established on the platform OGS was demonstrated. The method was verified by a benchmark test of solute transport in a one-dimensional homogeneous aquifer. We showed that the method can be adopted to simulate the process of retardation and decay as
well as advective-dispersive process. In addition, the method was extended to application in 3D porous media. The RWPT model produced the results in good agreement with the analytical solutions. It is well suited for the simulation of solute transport in saturated porous media. Furthermore, it can be used as a tool to observe the individual behavior of the solute mass with the post-processing.

With this fundamental, adapting the method to the simulation of solute transport in heterogeneous aquifer, coupled flow processes and multiphase flow are currently under development. The method will be applied in real field as well\cite{25}.

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REFERENCES


Influence of the size and amount of cork particles on the toughness of a structural adhesive

A.Q. Barbosa¹, L.F.M. da Silva², R.C. Carbas¹, Juana Abenojar³, Juan Carlos del Real⁴

¹IDMEC, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal
²Departamento de Engenharia Mecânica, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal
⁴Department of Mechanical Eng. Universidad Pontificia Comillas, C/ Alberto Aguilera 23. 28015 Madrid, Spain.

ABSTRACT

The inclusion of particles (nano or micro) is a method to improve the mechanical properties such as toughness of structural adhesives. Structural adhesives are known for their high strength and stiffness but also for their low ductility and toughness. There are many processes described in the literature to increase the toughness, being one of the most common the use of rubber particles. In the present study, natural micro particles of cork are used with the objective to increase the toughness of a brittle epoxy adhesive. The idea is for the cork particles to act like as a crack stopper leading to more energy absorption. The influence of the cork particle size and amount were studied. Particles of cork ranging from 38 to 250 µm were mixed in the epoxy adhesive Araldite 2020 from Huntsman. The amount of cork in the adhesive was varied between 1 and 5% in weight. Surface treatment (low pressure plasma) was applied to the cork powder to assess the effect of the interaction adhesive-cork with several degrees of adhesion.

Keywords: Adhesive, Cork, Surface treatment, Impact toughness

INTRODUCTION

Structural adhesives are often the best solution to join two components, in relation to traditional solutions, such as welding for example. One of the most common structural adhesive is the epoxy resin. The densely cross-linked molecular structure of structural adhesives is responsible for the good properties of these materials, but unfortunately it also makes them inherently brittle with poor resistance to crack initiation and propagation [1,2]. Structural adhesives are known for their high strength and stiffness but also for their low ductility and toughness. The ability of an adhesive to absorb energy without catastrophic failure can be increased through toughening of adhesives with a second phase. This results in enhanced
resistance to fracture with minimal change in the gross properties of the matrix resin [3]. The inclusion of particles (nano or micro) is a method to improve the mechanical properties such as toughness of structural adhesives [1]. There are many processes described in the literature to increase the toughness, being one of the most common the use of rubber particles [4]. However, natural materials are gaining attention as reinforcements of polymeric matrices due the thermal properties, low density, low cost and sustainability of the raw material [5]. Cork is a biological material with unique properties, produced by the cork oak. *Quercus suber L.* is the botanical name for a slow growing, evergreen oak that flourishes only in specific regions of the Western Mediterranean (Portugal, Spain, Southern France, part of Italy and North Africa) [4-6]. Portugal is the leadership of the world market relatively to this raw material, producing three-quarter of the total production. Cork may be described as a homogeneous tissue of thin-walled cells, regularly arranged without intercellular space. Cork has reveals an alveolar structure, similar to a honeycomb, without empty spaces between contiguous cells, which are therefore closed units [9].

These structural properties could be very useful to reinforce brittle resins, especially to improve the toughness as the closed cells could work to absorb the impact. However, the properties of a resin/cork composite are not only dependent of the materials properties, but also on their interfacial adhesion properties between the cork and the resin, size and amount of cork particles and mixing conditions [5]. Cork is hydrophobic due the suberin (main component of cork composition) and this fact could deteriorate the adhesion between cork particles and the epoxy resin. The hydrophobic properties could be altered using surface modification. There are several surface treatments to improve the cork-matrix adhesion with a positive effect on the mechanical properties of the composites [5]. Plasma treatment is one of the most versatile techniques in surface modification. Atmospheric pressure plasma is useful to activate the surface and improve the adhesion. This activation consists in grafting chemical functionalities on the surface in order to increase its surface energy. The plasma composition has influence on the treated material properties [10].

The cork particles should create obstacles to the propagation of the cracks thus increasing the toughness of the adhesive. Besides being apparently technically possible, this technique would also allow the use of this product (cork powder), which is not exploited by the cork industry that has an important impact in the Portuguese economy. Cork powder is generally burnt leading to unnecessary energy consumption and frequent accidents. The use of this material would give a new application perspective to the cork industry with potential benefits. Therefore, different amounts of cork and different particles sizes were included in a brittle epoxy to analyse the influence of these particles on the behaviour of cork/resin composite.
EXPERIMENTAL

1 - Materials

Cork powders, without any treatment, with different sizes (38-53 μm and 125-250 μm) were used. This cork powder was supplied by Amorim Cork Composites (Mozelos VFR, Portugal). The selected adhesive was Araldite 2020, from Huntsman Advanced Materials (Pamplona, Spain). This adhesive is a bicomponent (100/30 by weight), low viscosity (150mPa.s), transparent epoxy adhesive that cures at 100 ºC, during 15 minutes. The Young’s modulus of this adhesive is 3100 MPa, its tensile strength is 40.6 MPa and 5.8%.

This material was selected because it has a brittle behaviour, so the improvements on the toughness after the cork particles inclusion are easily seen.

2 – Manufacture of specimens

A homogeneous mixture of the cork powder in the resin must be assured to avoid the introduction of air bubbles and a uniform distribution of particles. The cork was mixed with the resin using a centrifuge mixing machine, SpeedMixer DAC 150™ (Buckinghamshire, UK), during 90 seconds at 1500 rpm. Specimens with and without cork were manufactured, with different surface treatment, different amount and cork particle size.

To assess the dispersion of the cork particles in the resin, thin layers of 5 μm which were cut by a microtome. Cork particles were coloured with methylene blue. A Leika Optic transmission microscope (OTM) was used.

3 - Surface treatments

Plasma treatment was used to modify the cork particles surface, since, depending on the selected gases, it can increase substantially the surface wettability and decrease the contact angle. The atmospheric plasma equipment used was a Plasma Treat GmbH (Steinhagen, Germany), which works in a frequency of 17 kHz and a high tension discharge of 20kV and a rotatory torch (1900 rpm). This system has a platform that allows to control of the treatment velocity automatically. These treatments were made at 8 mm from the surface and at 5m/min, on cork boards of 100x200x3 mm³. Figure 1 shows a scheme of the cork board used in the tests, with indication of the sections of the cork; radial section is represented by a “A”, tangential section by a “B” and axial or transverse section by a “C”.

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To measure the wettability of natural and treated cork, a goniometer OCA 15 (DataPhysics, Neurtek Instruments, Eibar-Spain) was used. To measure the contact angle, samples were placed in a chamber, at 25 ºC, saturated with water vapour.

4 - Density
The density of treated and untreated cork particles was measured using a helium pycnometer micromeritics AccuPyc 1330 de NEURTEK INSTRUMENTS (Spain).
The density of the impact test specimens was measured by Archimedes principle.

5 - Toughness impact test
To evaluate the impact toughness of the composite resin/cork several specimens were made varying the amount of cork, size of particles and surface treatment. Impact Charpy specimens according ASTM E23-02a were manufactured. Figure 2 shows the dimensions of machined specimens.

The toughness impact tests were made in a Rosand V1.01 machine. This test was made with a mass of 3.996 kg, at room temperature and with an initial velocity of 1.57 m/s. Three specimens were tested for each condition.

6 - SEM analysis
Scanning electron microscope (SEM) analyses were made in a JEOL JSM 6301F/ Oxford INCA Energy 350 / Gatan Alto 2500 microscope. This equipment was used to analyse cork particles.
before incorporation in the resin and to analyse the surface fracture of the composite after the impact tests.

RESULTS AND DISCUSSION

1 - Surface properties

Figure 3 and Table 1 show that with atmospheric plasma treatment the contact angle between cork surface and the water drop decreases. Table 1 show that the contact angle between water drop and the various cork surfaces does not vary substantially. This indicates that the adhesion of the cork particles will be uniform through the cork particles surface.

![Figure 3- Shape of the water drop in cork surface, without treatment (left) and with atmospheric plasma treatment (right).](image)

<table>
<thead>
<tr>
<th>Section</th>
<th>Treated specimen</th>
<th>Untreated Specimen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radial</td>
<td>30 ± 4</td>
<td>101 ± 11</td>
</tr>
<tr>
<td>Tangential</td>
<td>33 ± 7</td>
<td>99 ± 18</td>
</tr>
<tr>
<td>Axial</td>
<td>37 ± 2</td>
<td>103 ± 7</td>
</tr>
</tbody>
</table>

2 - SEM cork particles characterization

The cork particles size and shape were analysed in SEM. Figure 4 shows that particles with different sizes have different cell structures. Particles with 38-53 μm have a destroyed honeycomb cell structure, with several cells presenting an open structure and some just a single cell. On the other hand, particles with 125-250 μm size have a honeycomb structure composed by several cells, some open (edges of particles), but a few cells are closed (particle core).
Cork powder density changes with atmospheric plasma treatment. Figure 5 shows the density of cork particles with different sizes and treatments. The density decreases with plasma treatment. This effect may be because the plasma torch erodes part of cork surface. This increases the surface roughness, but leads to a weight loss.

Figure 5- Density of cork particles, with different sizes, untreated and with atmospheric plasma treatment.

3 - Toughness impact properties

Figure 6 shows the variation of the energy absorbed in the impact at load peak and at rupture. Figure 7 shows the displacement of the specimens during the test, in the two considered moments. It is notorious that the presence of cork influence the results. Specimens with 1% of untreated particles with 125-250 μm have a distinctive behaviour. These specimens show a better behaviour compared to the other composite specimens. They absorb more energy at rupture and give a higher displacement.
Figure 4 - Microstructure of cork powder; a) particles with 38-53 μm size, b) particles with 125-250 μm size.

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### Toughness Impact Properties

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Cork has good impact behaviour due to its cell structure disposition, giving a pillow effect. The cells compress, absorbing the impact. But if in the composite the particles do not have an intact cell structure, this effect disappears. Therefore, specimens with small particles are expected to have a worse behaviour than particles with 125-250 μm size. When in contact with resin, cork particles are surrounded by resin but the resin might not penetrate its core. Figure 8 shows images obtained with OTM and it can be seen that the core remains without resin; this was observed for all samples analysed. The behaviour of cork/resin composite is also influenced by the number of cells of the particle.
Figures 6 and 7 show that the plasma treatment gives worse results than untreated cork particles. This treatment improves the contact angle and the wettability, improving the adhesion between cork and resin. However, this treatment at the same time destroys part of the honeycomb structure of the cork cells. In addition, the cork particles damage can facilitate the resin penetration which could decrease the pillow effect of the cork, decreasing the energy absorption. If the resin penetrates inside of the cork cells, the specimen’s density should increase, compared to the specimen without cork. However, Figure 9 shows that the density variation is not substantial, considering the associated error. Therefore the interpretation may be regarded with caution.

Specimens with 1% of cork untreated particles (125-250 μm) presented the best combination of cork amount and particles size. Particles have an undamaged structure and work together with the resin and increasing the energy absorption of the composite.
4 - SEM surface fracture analysis

Figure 10 shows the fracture surface of a specimen without cork and a detail of fracture propagation.

Figures 11 and 12 show the fracture surface of specimens with 1% of cork particles of size 38-53 µm (treated and untreated respectively). These surfaces have a more brittle behaviour compared to that of the resin without cork because the surface is smoother.
Figures 12 and 14 show the fracture surface of specimens with 1% of cork particles with 125-250 μm size (treated and untreated respectively). In both figures, it is notorious that cork particles are empty (no penetration of resin), promoting energy absorption. These figures show that there is several crack planes close to the cork particles which indicates that cork is acting like an obstacle to crack propagation.
CONCLUSIONS

The influence of the size and amount of cork particles on the toughness of a structural brittle adhesive was evaluated by impact test and surface analyse. The following conclusions can be drawn:

- Atmospheric plasma surface treatment increases the contact angle and wettability of cork. There is an erosion of the surface which increased roughness, promoting adhesion between cork and resin. In cork particles, this surface treatment must be optimized. Cork wall cells are thin and if the treatment time or the distance of the torch are not the best, these walls can be destroyed. In future studies this effect must be analysed.

- SEM and OTM analysis show that most of cells are not filled with resin. The amount of cork, size of particles and surface treatments cause different fracture behaviours.

- Small amounts of cork particles with a structure composed by several cells and with well-preserved wall cells incorporated in a brittle resin present a better impact energy absorption than large amounts or small particles.

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REFERENCES


NUMERICAL MODEL BASED ON MESHLESS METHOD TO SIMULATE FSW

A.TIMESLI$^{1,2}$, H.ZAHROUNI$^{1}$, B.BRAIKAT$^{2}$, A.MOUFKI$^{1}$, H.LAHMAM$^{2}$

1 Université Paul Verlaine de Metz, Laboratoire d’Etude des Microstructures et de Mécanique des Matériaux, LEM3, UMR CNRS 7239, Ile du Sauley 57045, Metz Cedex 01 France.
2 Université Hassan II Mohammedia - Casablanca, Faculté des Sciences Ben M’sik, Laboratoire de Calcul Scientifique en Mécanique, Casablanca, Maroc.

Key words: FSW, Simulation, Meshless, SPH

Abstract. In the present work, a numerical models based on the meshless method “the smoothed particle hydrodynamics (SPH)” is developed to simulate the Friction Stir Welding (FSW). This technique type is well adapted to modeling of mixing zone which is subjected to high strain rate. We limit ourselves to two dimensional problems.

1. INTRODUCTION

Friction Stir Welding (FSW) was invented by the British Welding Institute TWI since 1990s for aluminum sheets [1]. The main advantage of this technique is its ability to joining in solid state a class of metal alloys which are generally difficult to weld by conventional welding processes. Joining two workpieces by FSW consists in heat generation due mainly to the shoulder and material mixing thanks to the pin. Heat is generated two main mechanisms, friction and plastic dissipation [2-4].

Numerical modeling of FSW has been investigated by several authors considering thermal or thermo-mechanical framework. Different formulations have been proposed in these contributions concerning Eulerian, Lagrangian or Arbitrary Lagrangian Eulerian formulations [5-9]. The choice of a specific formulation is mainly oriented by the relevant phenomenon that authors have to analyze. In the face of the numerous industrial applications of FSW process, its development remains largely empirical and based on and based on a large experimental knowledge of the process. Experimental works are very numerous. The numerical simulations also but the treatment of mixing remains a major difficulty for the numerical analyst. The numerical modeling of FSW has been investigated by several authors considering thermal or thermomechanical framework. Different formulations have been proposed in these contributions concerning Eulerian, Lagrangian or Arbitrary Lagrangian Eulerian formulations. The choice of a specific formulation is mainly oriented by the relevant phenomenon that authors have to analyze. The mixing is difficult to achieve using the finite element method because the area near the welding tool is the seat of large deformations. For this, we propose in this work using the meshless methods.

In this work, a numerical model based on the smoothed particle hydrodynamics SPH [10-14]
method is developed to simulate the Friction Stir Welding. This model considers a non
Newtonian fluid near the tool region using a thermomechanical constitutive law.

The main advantage of this technique concerns that the material mixing around the tool which
is very difficult or impossible to achieve with other numerical methods such as finite element
method. The history of the particles is available; one can obtain the residual stresses.

For plates of large sizes, the mixing zone rest very localized. This is the area where the strains
are very large and generate a source of intense heat. Entire plate contributes to heat exchange
with the outside environment. One idea is to treat the localized area near the tool so different
from the rest of the plate. We propose in this work using a technique based on meshless
method to model the mixing of material around the tool.

2. SPH MODEL FOR 2D SIMULATION OF FRICTION STIR WELDING

2.1. GOVERNING EQUATIONS

The different equations needed to simulate the Friction Stir Welding process by SPH are
given by the conservation laws including:

First, the mass conservation:

\[ \frac{dp}{dt} = -\rho \nabla \cdot \mathbf{v} \]  

(36)

The second equation describes the classical momentum conservation:

\[ \frac{dv}{dt} = \frac{1}{\rho} \nabla \sigma \]  

(37)

The third equation is energy conservation:

\[ \rho c_p \frac{dT}{dt} = \nabla \cdot (k \nabla T) + q_v \]  

(38)

The rate of heat generation due to plastic deformation is given by:

\[ q_v = -\beta (\tau : \nabla \mathbf{v}) \]  

(39)

where \( \beta \) represent the fraction of mechanical energy transformed to heat and is assumed to
be 0.9 [15].

The stress tensor is given by:

\[ \sigma = -pI + \tau \]  

(40)

Where \( p \) is the hydrostatic pressure, \( I \) the identity tensor and \( \tau \) the deviatoric stress tensor:

\[ \tau = \mu [\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3}(\nabla \cdot \mathbf{v})I] \]  

(41)

Viscosity of the particles decreases with increasing temperature according to:

\[ \mu = A \left( 1 - \left( \frac{T - T_{ref}}{T_{melt} - T_{ref}} \right)^m \right) \]  

(42)

A and \( m \) are material parameters. \( T_{ref} \) is a reference temperature and \( T_{melt} \) is the melting
temperature. The pressure is obtained using the equation of state:
P = c^2 \rho

c is the speed of sound.

2.2. PRINCIPLE OF SPH METHOD

The SPH method is based on an integral approximation [11]:

\[ f(\vec{r}) = \int f(\vec{r}') W(\vec{r} - \vec{r}', h) d\vec{r}' \]

Where h is the smoothing length and W is the kernel function. The approximate forms of the integral by SPH:

\[ f(\vec{r}_a) = \sum_{b=1}^{N_p} \frac{m_a}{\rho_b} f_b \left( \|\vec{r}_a - \vec{r}_b\|, h \right) \]

\[ \nabla f(\vec{r}_a) = \sum_{b=1}^{N_p} \frac{m_a}{\rho_b} (f_a - f_b) \left( \|\vec{r}_a - \vec{r}_b\|, h \right) \]

Where \( m_b, \rho_b \) et \( N_p \) are the mass, the density of the particle and the number of neighboring particles respectively. Example: kernel function type cubic spline [16]:

\[ W(\|\vec{r}_a - \vec{r}_b\|, r, h) = \alpha_d \times \begin{cases} 
1 - \frac{3}{2} q^2 + \frac{3}{4} q^3 \text{ si } q \leq 1 \\
\frac{1}{4} (2 - q)^3 \text{ si } 1 \leq q \leq 2 \\
0 \text{ si } q \geq 2
\end{cases} \]

With \( q = \frac{\|\vec{r}_a - \vec{r}_b\|}{h} \)

And \( \alpha_d = \begin{cases} 
10/(7\pi h^2) \text{ en } 2D \\
1/(\pi h^3) \text{ en } 3D
\end{cases} \)

2.3. SPH FORMULATION AND TIME DISCRETIZATION

Using SPH approximations of functions and its spatial derivatives the governing equations are discretized resulting in a set of ordinary differential equations:

\[ \frac{d\rho_a}{dt} = \sum_{b=1}^{N_p} m_b \vec{v}_{ab} \vec{v}_a W_{ab} \]

\[ \frac{d\vec{v}_a}{dt} = \sum_{b=1}^{N_p} m_b \left( \frac{P_a}{\rho_a^2} + \frac{P}{\rho_a^2} + \Pi_{ab} \right) \vec{v}_a W_{ab} + \sum_{b} \frac{4 m_b \mu_a \mu_b}{\rho_a \rho_b (\mu_a + \mu_b)} \frac{(\vec{v}_a - \vec{v}_b)(\vec{r}_a - \vec{r}_b) \vec{v}_a W_{ab}}{(\vec{r}_a - \vec{r}_b)^2} \]

\[ C_{v,a} \left( \frac{dT}{dt} \right)_a = \sum_{b} m_b \frac{4 k_a k_b}{\rho \rho_b (k_a + k_b)} (T_a - T_b) \frac{(\vec{r}_a - \vec{r}_b) \nabla W(r_a - r_b, h)}{(\vec{r}_a - \vec{r}_b)^2} + q_v \cdot \vec{h} (T_a - T_{col}) \]
\[ q_e = \beta \sum_{b} \frac{2m_b \mu_a \mu_b}{\rho_a \rho_b (\mu_a + \mu_b)} \frac{[(\vec{v}_a - \vec{v}_b).\vec{(r}_a - \vec{r}_b)]^2 (\vec{r}_a - \vec{r}_b)}{(\vec{r}_a - \vec{r}_b)^2} \vec{v}_a W_{ab} \]  

(51)

\[ \mu_a = A \left( 1 - \left( \frac{T_a - T_{ref}}{T_{melt} - T_{ref}} \right)^m \right) \]  

(52)

\[ p_a = c^2 \rho_a \]  

(53)

### 2.3.1. BOUNDARY CONDITIONS

To avoid penetration of the particles representing weld material into the tool, boundary particles are forced to satisfy the same equations as fluid particles. Thus, they follow the momentum equation, the continuity equation, the equation of state, and the energy equation. However, they do not move according to the XSPH variant. They move together with velocities:

\[ \vec{v}_i = \vec{r}_{i,t} \omega + \vec{v}_i, \vec{r}_{i,t} = (x_i - x_c, z_i - z_c, 0), \]  

(54)

Where \( \omega \) is the rotational velocity and \( v_i \) is the translational velocity of the tool. \( x_c \) and \( z_c \) are coordinates of the tool rotation axis. When a fluid particle approaches a boundary the density of the boundary particles increases according to the continuity equation (Eq. 48) resulting the increasing pressure following the equation of state (Eq. 53). Thus, the force applied on the fluid particle increases due to the pressure term \( (P/\rho^2) \) in momentum equation (Eq. 49). When the distance between the boundary particle and the fluid particle becomes smaller than 2h, the density, pressure and force applied on the incoming particle increase generating the repulsion mechanism.

### 2.3.2. TIME DISCRETIZATION SCHEME

The time scheme to deal with the derivatives in time is the explicit “velocity Verlet” algorithm [17] as follows:

\[ \vec{v}^{n+1}_a = \vec{v}^n_a + 0.5\Delta t (\vec{F}^n_a + \vec{F}^{n+1}_a); \rho^{n+1}_a = \rho^n_a + 0.5\Delta t (D^n_a + D^{n+1}_a) \]  

\[ \vec{r}^{n+1}_a = \vec{r}^n_a + \Delta t \vec{v}^n_a + 0.5\Delta t^2 \vec{F}^n_a; T^{n+1}_a = T^n_a + 0.5\Delta t (E^n_a + E^{n+1}_a) \]  

(55)

With \( \frac{d\vec{v}}{dt} = \vec{F}_a, \frac{d\rho_a}{dt} = D_a, \frac{d\vec{r}^2}{dt} = \vec{v}_a, \frac{dT}{dt} = E_a \)

### 2.4. NUMERICAL DISCUSSION

We consider a plate made of aluminum alloy with L=50 mm length and a width of 20 mm (see Figure 4). The parameters of the law (Eq. 52) are defined as follows: \( A = 200 \) Mpa.s\(^{-1}\), \( m=1 \), \( T_{ref} = 25^\circ C \), \( T_{melt} = 502^\circ C \). The tool is rigid and made of steel material with cylindrical geometry (\( r_p=2.5 \) mm rayon). The physical properties (material conductivity \( k \), specific heat \( C_p \), and density \( \rho \)) used for aluminum plate are presented on table 1.
2.3.1. BOUNDARY CONDITIONS

To avoid penetration of the particles representing weld material into the tool, boundary particles are forced to satisfy the same equations as fluid particles. Thus, they follow the momentum equation, the continuity equation, the equation of state, and the energy equation. However, they do not move according to the XSPH variant. They move together with velocities:

\[
\frac{\rho_m}{\rho_0} \left( \mathbf{x} - \mathbf{x}_0 \right) = \mathbf{v}_m + \mathbf{v}_t - \mathbf{v}_c - \mathbf{v}_z
\]

Where \( \mathbf{v}_m \) is the rotational velocity and \( \mathbf{v}_t \) is the translational velocity of the tool. \( \mathbf{v}_c \) and \( \mathbf{v}_z \) are coordinates of the tool rotation axis. When a fluid particle approaches a boundary the density of the boundary particles increases according to the continuity equation (Eq. 48) resulting in an increasing pressure following the equation of state (Eq. 53). Thus, the force applied on the fluid particle increases due to the pressure term in the momentum equation (Eq. 49). When the distance between the boundary particle and the fluid particle becomes smaller than 2h, the density, pressure and force applied on the incoming particle increase generating the repulsion mechanism.

2.3.2. TIME DISCRETIZATION SCHEME

The time scheme to deal with the derivatives in time is the explicit “velocity Verlet” algorithm [17] as follows:

\[
\begin{align*}
\mathbf{x}_{n+1} &= \mathbf{x}_n + \mathbf{v}_n \Delta t + \frac{1}{2} \mathbf{a}_n \Delta t^2 \\
\mathbf{v}_{n+1} &= \mathbf{v}_n + \mathbf{a}_n \Delta t
\end{align*}
\]

Where \( \mathbf{a}_n = \frac{\mathbf{F}_n}{m} \) is the acceleration.

Tableau 1: Physical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
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<tbody>
<tr>
<td>( \rho ) (kg/m(^3))</td>
<td>2780</td>
</tr>
<tr>
<td>( C_p ) (J/K.kg)</td>
<td>875</td>
</tr>
<tr>
<td>( k ) (W/m.K)</td>
<td>140</td>
</tr>
</tbody>
</table>

In the proposed work, we have used a heat transfer coefficient \( h_{\text{Lat}} = 30 \, \text{W/m}^2\cdot\text{K} \), a ambient temperature \( T_0 = 25\, ^\circ\text{C} \), a welding velocity of 2 mm/s and a rotation speed of 20 rad/s.

![Figure 4: Geometry and boundary conditions of FSW configuration treated by SPH](image)

![Figure 5: Mixing of particles around the welding tool by SPH](image)

Table 1: Physical properties

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</table>

Figure 4: Geometry and boundary conditions of FSW configuration treated by SPH

Figure 5: Mixing of particles around the welding tool by SPH
Figure 5 presents the figures of mixing of material for different computing time; these figures represent the positions of discrete dots of material. This result shows the advantage of the SPH method to simulate industrial processes involving large deformation such as FSW process. The distribution of the temperature field is shown in Figure 6.

![Temperature distribution](image)

**Figure 6:** Temperature distribution equivalent to the mixing of configurations of figure 2

The results of our approach are compared with those obtained using the Fluent software. This code is based on an Eulerian formulation and a finite volume discretization. To validate the results of our algorithm, we choose two equivalent configurations between the two formulations Lagrangian and Eulerian (Figure 4 and 7). The SPH calculation is performed until the tool reaches the plate center. This computation needs a time $t = t_c = 9\text{s}$. In the eulerian formulation, unsteady calculation with a time $t_c$ is performed (Figure 8). The two calculations use the same constitutive law (Eq. 52). Figure 10 and 11 shows the comparison between SPH and Fluent of temperature evolution along the horizontal and vertical section (see Figure 9) using kernel function type Gaussian. One can observe that a relative error of at least 2% is obtained confirming the relevance of the proposed algorithm.
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Figure 7: Geometry and boundary conditions of FSW configuration treated by Fluent

Figure 8: Temperature distribution by Fluent

Figure 9: Horizontal section (A-A) and vertical section (B-B)
2.5. FSW SIMULATION

In the following, and after validation of the model, we propose a more realistic constitutive law. Furthermore, we propose a model coupling that will allow the simulation of welding of large plates. A local model that will simulate the mixing around the welding tool is coupled to a thermal model that takes into account the entire structure and its environment. It does not take much time because the search of neighbors is done once only for the thermal model.

2.5.1. CONSTITUTIVE LAW

The constitutive relation is chosen in this form:
\[
\mu(T, \tilde{\varepsilon}) = \frac{\sigma}{3\tilde{\varepsilon}} \tag{22}
\]

Where \( \tilde{\varepsilon} \) is the equivalent strain rate, and \( \bar{\sigma} \) is the von Mises equivalent stress given by:

\[
\bar{\sigma} = \frac{1}{\alpha} \sinh^{-1}\left(\frac{Z(\tilde{\varepsilon}, T)}{A}\right)^{\frac{1}{n}} \tag{23}
\]

Which \( Z(\tilde{\varepsilon}, T) \) represents the Zener-Hollomon parameter:

\[
Z(\tilde{\varepsilon}, T) = \tilde{\varepsilon} \exp\left(\frac{Q}{RT}\right) \tag{24}
\]

Where \( Q \) is the activation energy, \( R \) the gas constant, and \( n \) are material parameters given in reference [18].

### 2.5.2. RESULTS

We consider a plate made of aluminum alloy (aluminum 6061) with 90 mm length and a width of 60 mm. The mechanical and thermal characteristics are given in the following table:

<table>
<thead>
<tr>
<th>( \rho ) (kg/m(^3))</th>
<th>( C_p ) (J/K.kg)</th>
<th>( k ) (W/m.K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2780</td>
<td>980</td>
<td>140</td>
</tr>
</tbody>
</table>

**Tableau 2:** mechanical and thermal characteristics

In the present work, we use a heat transfer coefficient \( h_{lat}=17 \) W/m\(^2\).K, an ambient temperature \( T_0=25^\circ\text{C} \), a welding velocity of 2 mm/s and a rotation speed of 20 rad/s.

![Figure 12: Mixing of particles](image)

Figure 12 presents the mixing of material at \( t = 9s \); this figure represents the positions of discrete dots of material. The distribution of the temperature field is presented in Figure 13.
Figure 14 and 15 show the temperature evolution along the horizontal and vertical section (see Figure 9) using kernel function type Gaussian.
3. CONCLUSION

Material mixing is very difficult or impossible to achieve with other numerical methods such as finite element method because material zone located near the welding tool is subjected to high strain gradient and remeshing procedure is often necessary.

In this contribution, we have proposed a first model based on SPH to model FSW process. The main advantage of this technique concerns that the material mixing around the tool. The history of the particles is available; one can obtain the residual stresses.

REFERENCES


PARTICLE-FILLED DENTAL COMPOSITE: SHRINKAGE INDUCED RESIDUAL STRESSES AND OVERALL MECHANICAL PROPERTIES

ONDŘEJ PREJZEK*, TOMÁŠ MAREŠ *
* Department of Mechanics, Biomechanics and Mechatronics
Faculty of Mechanical Engineering, Czech Technical University in Prague
Technická 4, 16607 Prague, Czech Republic
e-mail: ondrej.prejzek@fs.cvut.cz, http://mechanika.fs.cvut.cz/

Key words: Dental Composite, Polymerization Shrinkage, Residual Stress, FEM.

Abstract. This work is focused on numerical simulation of the shrinkage phenomenon and its influence on overall elastic modulus of the composite and it is supported by experimental verification of results. It has been motivated by experimentally observed discrepancy between elastic moduli in uniaxial compression and tension. Its main contribution is a hypothesis linking this discrepancy with the mentioned phenomenon of polymerization shrinkage. The residual stress field after shrinkage is computed and its effect on the tangent stiffness of certain material points is discussed. The finite element model is built in a parametric manner with varying volume fraction and distribution of particles. To simplify the irregular distribution of particles in the composite, the model employs a crystallographic analogy of lattices. The plasticity model used to simulate resins behaviour has critical influence on the results. It is hypothesized, that the residual stresses beyond the yield stress weaken the model response in the compressive direction. Presented hypothesis is proven using the simplest von Mises criterion and further explored using the more realistic Drucker-Prager criterion.

1 INTRODUCTION

Advanced dental materials belong to most common applications of particle reinforced composites. They consist from glass particles and polymer resin. Dental composites are used for their superior aesthetic properties and resistance to environment. However their mechanical properties, namely strength and resistance to fracture, still require to be enhanced. It is hypothesized, that certain mechanical properties are influenced by residual stresses developed due to polymerization shrinkage.

In order to predict fracture and obtain optimal shape of restoration to preclude its development, realistic modeling of the physical process of shrinkage and its effect on mechanical properties becomes critical.

Polymerization of the composite’s resin causes its shrinkage, as the monomers are linked into chains [1, 2] which occupy smaller space. As the resin and entire composite material shrinks, internal residual stresses occur. Most of the literature, related to dental materials, investigates macroscopic stresses, developed in the composite, constrained by a tooth [3, 4]. There, the composite is considered to be homogenous material. Development of curing residual stresses on the interface between the filler and resin has been studied for ceramic-metal composites [5]. The influence of fiber arrangement in CFRP (carbon-fiber...
reinforced polymer) has been investigated [6], using the finite element method (FEM). Residual stresses in composite materials, occurring during polymerization, influence mechanical properties, such as strength [7], plastic behavior [8] or resistance to damage initiation and development [9].

During recent research on particle filled dental composites, discrepant values of Young’s modulus have been observed, depending on applied measurement method. Tensile moduli are referred to reach values over 10 GPa, flexural moduli to be 6-8 GPa, and compressive moduli to be 3-5 GPa [10,11,12]. Elastic modulus of a composite, consisting of polymer resin (Ethoxyl-BPDMa, TEGDMA, Bis-GMA) and glass particles (SiO₂, BaO, B₂O₃, Al₂O₃) has been measured [13]. Results show significantly higher elastic modulus under uni-axial tension, than under uni-axial compression, although both particles and resin have equal modulus in both directions and yield strength of resin is higher under the compressive load (figure 1).

![Stress-strain curves of composite (left) and resin (right)](image)

This work tries to investigate a possible link between the polymerization, development of the residual stresses and the discrepancy between the elastic moduli under tensile and compressive direction.

2 NUMERICAL MODEL

The shrinkage process, development of residual stresses, and its influence on the overall response has been simulated using software ABAQUUS. The amount of linear polymerization shrinkage of resin is referred to be up to 7% [2]. In the FE model, the shrinkage process has been mimicked by a thermal analogy. Regions occupied by resin have been prescribed coefficient of thermal expansion (CTE) of 7%, while CTE of particles is 0. The shrinkage strain, and consequently residual stress field, is introduced in the first step of analysis, by decrease of temperature by 1K. From second step of the analysis, external load in uni-axial compressive and tensile direction is applied, to simulate the test. Load is applied in 12 steps displacement of ∆l/l by 0,05% in each, up to ∆l/l=0,6%, what is behind the point, where the composite material breaks under tensile load in the experiments (figure 1).

In nature, the microstructure of the composite is irregular in size, shape and distribution of
particles. In the model, particles are spherical, and its distribution is simulated by three crystallographic lattices, cubic, body-centered cubic (BCC) and face-centered cubic (FCC). For each lattice, simulation of five models is carried out, with mutual distance of particles varying from 1 to 20% of their diameter, while the volume fraction of particles reaches values from 30.3% (cubic array-20% gap) to 71.8% (FCC array – 1% gap). The microstructure is assumed to be periodical and is simulated by a Representative Volume Element (RVE) with defined periodical boundary conditions. To mesh the investigated microstructural unit, linear tetrahedral elements have been chosen for their low computational cost. The applicability of this particular element has been confirmed by an analysis of element-type.

The modeled components of the composite material are polymer resin with an elastic modulus of 2.6 GPa and hollow glass particles with elastic modulus of 70 GPa. According to observations in [5], resin shows asymmetric yielding behavior with the initial yield stress of 20 MPa in tension and 50 MPa in compression, as can be seen in the Figure 1. Particles are considered to be perfectly linearly elastic. In first series of simulations, von Mises criterion, based on the lower (tensile) branch of the stress-strain curve has been applied. In the second one, the more realistic pressure-dependent Drucker-Prager criterion has been introduced.

3 RESULTS

3.1 Stress and strain distribution after curing – von Mises model

Distribution of stress and strain after polymerization curing has been studied. The distribution of residual stress (Figures 3,5,6) shows, that significant part of stress field is of a tensile nature, and only limited areas are compressed, in the sense of negative values of σ_{11}, σ_{22}, σ_{33}. If compared with the strain distribution (Figure 3), compressed are the regions, where the negative strain is higher than the value of shrinkage strain (7%). From Figure 4., development of plastic states can be observed. Compressed regions in narrow gaps between particles are highly plastic, while stretched regions remain elastic, or slightly plastic.
Figure 3: FCC Array-2\% gap, von Mises material model: Distribution of $\sigma_{22}$ after curing.

Figure 4: FCC Array-2\% gap, von Mises material model: Areas with strain over the value of shrinkage-caused strain.

Figure 5: FCC Array-2\% gap, von Mises material model: Elastic regions ($\sigma_{\text{eff}} < 50$ MPa) after curing.
3.2 Overall stress-strain response – von Mises model

The overall elastic modulus has been studied for each of the particle distribution arrays. Uni-axial tensile and compressive experiments have been simulated and resulting stress-strain curves (Figure 7.) have been compared with the results of experimental measurement. In the case of von Mises material model, for each of modeled arrays, the tensile stress-strain curve is higher than the compressive one, but the ratio of tensile ($E_t$) and compressive elastic modulus ($E_c$) does not reach the experimentally observed value. For each particular model, the $E_t/E_c$ ratio is between 1.2 and 1.6 and the filler distribution does not tend to have influence on the ratio. Both tensile and compressive elastic moduli, by each of distribution arrays, tend to rise with the filler content. Except those models with very low filler content, all stress-strain curves are between the experimentally measured curves, and are closer to the curve of compressive experiment.

![Figure 6: FCC Array-2% gap- Plastic regions (50MPa < σ_{eff} < 58 MPa) after curing.](Image)
Figure 7: Stress-strain curves - Parametric simulation compared with experimental data, von Mises material model

Figure 8: Stress-strain curves: Element type sensitivity (FCC-gap/particle diameter = 0.1)

Figure 8. shows the influence of chosen finite element on the results of stress-strain simulation. Linear and quadratic tetrahedral elements of various mesh density have been subjected to the analysis, as well as an element with hybrid formulation. The difference of elastic moduli in one direction does not exceed 10%, and affects both curves in the same manner, so the $E_t/E_c$ does not significantly change. These results allow the use of linear tetrahedral elements, which have lowest demand for CPU time.

3.3 Stress and strain distribution after curing – Drucker-Prager model

Distribution of residual stress by the Drucker-Prager material model (Figure 7.) is of similar nature as observed by the von Mises model, while the plastic (in terms of the compressive stress-strain curve-Figure 1.) compressed regions are smaller (Figure 8.).
Figure 9: FCC Array-2% gap Drucker-Prager material model: Distribution of $\sigma_{22}$ after curing.

Figure 10: FCC Array-2% gap, von Mises material model: Elastic regions ($\sigma_{\text{eff}} < 80$ MPa) after curing.

Figure 11: FCC Array-2% gap, von Mises material model: Plastic regions ($80$ MPa < $\sigma_{\text{eff}} < 88$ MPa) after curing.
3.4 Overall stress-strain response – Drucker-Prager model

The stress-strain curves resulting from the simulation with the Drucker-Prager material (Figure 9.) do not capture the experimentally observed discrepancy of tensile and compressive moduli. At lower stress levels, the curves are close to equal, or the tensile curves are slightly higher. At higher stress levels, the tensile curves tend to be lower than the compressive ones. Resulting moduli are also higher than those of simulation with the von Mises material.

![Cubic Array - Drucker Prager](image1)

![BCC Array - Drucker Prager](image2)

![FCC Array - Drucker Prager](image3)

**Figure 12:** Stress-strain curves - Parametric simulation compared with experimental data, Drucker-Prager material model

4 DISCUSSION

All investigated models show similar distribution of stress in resin. In major part of resin, namely in large regions, the stress field is of tensile nature (Figure 3). Particles trying to move towards each other, due to shrinkage, are constrained by the shrinkage strain from the other side of particle, and the shrinking resin is stretched. In the regions of narrow gaps between particles, the particles moving towards each other compress the resin by more than the 7% of polymerization shrinkage. This causes the compressive stress in these regions. Similarity between stress distribution and plasticity development can be seen (Figure 3., 5. and 6.). Compressed regions are highly plastic, while stretched regions are elastic, or only slightly
plastic. This fact mainly contributes to the discrepancy of tensile and compressive moduli. If the plastic, compressed regions are subjected to further compressive load, they respond with tangent modulus close to zero, while under tensile unloading their tangent modulus is equal to the initial elastic modulus. The tangent modulus of the tensile regions remains unchanged, elastic. Applying any mixing law, the resulting compressive modulus is lower than the tensile one. By the Drucker-Prager material model, the higher yield strength in compressive direction allows only small regions to become fully plastic, and smaller regions do not influence the model in that scale as by the von Mises model. This causes the minimal difference between $E_t/E_c$. The discrepancy between $E_t$ and $E_c$ can be better captured after implementation of the stress relaxation into the model. The tangent modulus of polymer resin after relaxation from plastic stress values is assumed to be close to zero under further loading and quasi-elastic under unloading. Then the compressed regions, with lower (relaxed) stress values must be larger to ensure equilibrium in the model, and they will contribute more to the weakening of the material in the compressive direction.

5 CONCLUSION

Presented study shows the influence of residual stresses on mechanical properties of the investigated composite. Origin and nature of residual stress in particular regions of resin is explained as well as its effect on the overall elastic modulus. The highly plastic nature of the residual stresses requires an accurate model of plastic behavior. The simplest plasticity model, the von Mises criterion, shows how the residual stresses affect the composites behavior. The Drucker-Prager criterion is more suitable for modeling of polymers. In this particular case, it does not match the results and it needs to be enhanced by a stress relaxation model. In the future, stress relaxation properties of the resin will be measured and the data will be used to develop its visco-elastoplastic constitutive model.

ACKNOWLEDGEMENT

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REFERENCES

ENRICHED CONVECTED PARTICLE DOMAIN INTERPOLATION (CPDI) METHOD FOR ANALYZING WEAK DISCONTINUITIES

ALIREZA SADEGHIRAD*, REBECCA M. BRANNON* AND JAMES GUILKEY†

*Department of Mechanical Engineering
University of Utah
50 S. Central Campus Dr., Salt Lake City, UT 84108, USA
e-mail: alireza.sadeghirad@utah.edu and rebecca.brannon@utah.edu
web page: http://www.mech.utah.edu/brannon/

†Schlumberger Technology Corporation
14910 Airline Road, Rosharon, TX 77583, USA
e-mail: james.guilkey@utah.edu
Web page: http://www.mech.utah.edu/people/faculty/guilkey.html

Key words: Convected Particle Domain Interpolation, Material Point Method, Enrichment Techniques, Weak Discontinuities.

Abstract. Convected particle domain interpolation (CPDI) is a recently developed technique for more accurately approximating material point method (MPM) integrals by replacing the shape functions with interpolations of the shape functions to corners of particle domains that are tracked as parallelograms in 2-D (or parallelepipeds in 3-D). In this paper, the CPDI method is enhanced to (1) more accurately track particle domains with very little computational overhead in comparison to the original CPDI, (2) remove gaps/overlapping between particle domains, and (3) give more flexibility in choosing particle domain shape in the initial configuration. This enhanced CPDI method is then enriched to accurately solve weak discontinuities in the displacement field across a material interface that passes through the interior of a grid cell. The new enriched CPDI2 method is demonstrated using one- and two-dimensional examples.

1 INTRODUCTION

The Material Point Method (MPM) [1, 2] and the closely related Generalized Interpolation Material Point (GIMP) method [3] have been successfully used in simulation of some complicated engineering problems (see for example [4, 5, 6, 7, 8, 9]). Like many other particle methods, both MPM and GIMP gain computational efficiency by solving
the governing equations on a background grid that can be retained or reset at the end of each time step, while field data are stored at moving Lagrangian particles. The conventional MPM, which considers each particle as a lumped mass, is well known to suffer from a “cell crossing instability” in large deformation problems caused by a jump discontinuity in the gradient of low-order shape functions across cell boundaries. The GIMP method eliminates this error by replacing point evaluation of the MPM integrals with a weighted average of the integrand over a finite domain in the neighborhood of the particle.

The GIMP weight, or characteristic, function is typically chosen to be a “top-hat” function that is equal to unity within a finite domain centered around the particle, and zero elsewhere. The standard MPM formulation is exactly recovered when the choice of characteristic function is the Dirac delta function. For large deformation problems, the GIMP method gains accuracy if particle domains are allowed to deform with the material. Some early efforts to evolve particle domains with deformation only allowed rectangles (or cuboids in 3-D) to change dimension but not shape. However, a first-order accurate description of domain convection must allow rectangles to deform to parallelograms (parallelepipeds in 3-D) [10]. With a conventional GIMP formulation using a top-hat function, tracking particle domains as parallelograms is prohibitively costly because of a need to divide these parallelograms over cell boundaries to account for the changes in the shape functions across cell boundaries. The convected particle domain interpolation (CPDI) method [10] circumvents this problem by replacing the grid shape function with an alternative function that is an interpolation of the original shape function to the corners of the particle domain. Since the CPDI alternative shape function is smoothly varying over the particle domain, the revised MPM integrals may be evaluated analytically. In the original CPDI method, now called CPDI1, the particle domains were approximated to be parallelograms (or parallelepipeds in 3-D). An enhancement, called CPDI2, describes particle domains by quadrilaterals (or hexahedra in 3-D). Advantages of CPDI2 over CPDI1 include (1) more accurately tracking particle domains with very little computational overhead in comparison to CPDI1, (2) removing gaps/overlapping between particle domains, and (3) giving more flexibility in choosing particle domain shape in the initial configuration. Like CPDI1, the CPDI2 method describes fields over particle domains based on values of those fields mapped to the particle domain’s corners.

In the MPM techniques, spurious non-monotonic variation in stress can occur at material interfaces passing through the interior of a grid cell. This problem is caused by low-order shape functions being incapable of describing the jump in displacement gradients needed to allow the compliant materials to experience larger strain than stiff material in the same cell. The CPDI2 method can rectify this shortcoming by supplementing the nodal degrees of freedom already defined on the background grid with the corner values of the fields at particles near a material interface. This approach provides enrichment capable of properly describing weak discontinuities in the displacement field (i.e., strong discontinuities in strain) across a material interface that passes through the interior of a grid cell. For clarity, this approach will be first demonstrated in a simple 1-D context,
where spurious stress spikes and dips caused by incorrect partitioning of deformation within a cell are eliminated through CPDI2 enrichment, thus giving results comparable to a traditional Lagrangian finite-element simulation that has a node at the material interface. Recognizing that particle methods are adopted in situations for which traditional Lagrangian finite elements or Eulerian finite difference methods are unsatisfactory, improvements in accuracy of CPDI2 over CPDI1, and even more dramatic improvements in comparison to legacy methods of evaluating non-advecting GIMP integrals, are presented.

The paper is organized as follows: Section (2) introduces the basic strategy of the material point methods. Section (3) presents the enhanced version of the original CPDI method. The enrichment technique for this enhanced version is explained in Section (4), followed by the numerical examples in Section (5). Finally, Section (6) draws some conclusion remarks.

2 REVIEW OF THE MPM TECHNIQUES

In this section, formulations of the conventional MPM, GIMP, and CPDI methods are presented based on the “update stress last (USL)” algorithm described by Bardenhagen [11]. In the MPM, particle mass and momentum are mapped to the grid nodes at the first of each time step.

\[
m_i = \sum_p \varphi_{ip} m_p
\]

\[
v_i = \frac{\sum_p \varphi_{ip} m_p v_p}{m_i}
\]

in which \(m_i\) and \(v_i\) are mass and velocity at grid node \(i\), \(m_p\) and \(v_p\) are mass and velocity at particle \(p\), and \(\varphi_{ip}\) can be viewed as the average of the \(i\)th grid shape function, \(S_i\), over the \(p\)th particle,

\[
\varphi_{ip} = \frac{1}{V_p^*} \int_{\Omega_p^*} \chi_p(x - x_p) S_i^*(x) dx
\]

in which \(\chi_p(x)\) and \(\Omega_p\) are the particle characteristic function and its support-domain of volume \(V_p^*\) respectively, and \(S_i^*\) is the shape function or, for CPDI, the alternative shape function. In the MPM, the characteristic function is chosen as the Dirac delta function and a “top-hat” characteristic function is typically used in the GIMP method:

\[
\chi_p(x) = \begin{cases} 
1 & x \in \Omega_p^* \\
0 & \text{otherwise}
\end{cases}
\]

Whereas \(\Omega_p\) has been selected to be rectangular (or cuboid in 3-D) in legacy GIMP formulations, CPDI formulations are well suited to taking \(\Omega_p\) to be a better approximation to the Voronoi cell \(\Omega_p\) associated with the particle.

In the MPM, the discretized weak form of the equations of motion,

\[
m_i \ddot{a}_i = f^\text{int}_i + f^\text{ext}_i
\]
is solved at each time step. Here,

\[ f_{\text{int}}^i = - \int_{\Omega} \nabla S_i \cdot \sigma d\Omega, \quad (6) \]

and

\[ f_{\text{ext}}^i = \int_{\Omega} \rho S_i b d\Omega + \int_{\Gamma^t} S_i \tau d\Gamma, \quad (7) \]

in which \( \nabla S_i \) is the grid shape function gradient, \( b \) is the body force per unit mass, and \( \Gamma^t \) is the part of the problem domain boundary where the prescribed traction \( \tau \) is applied.

The integral in Eq. (6) is broken into the sum of integrals over elements in the FEM, whereas the MPM breaks the integral over particle domains as

\[ f_{\text{int}}^i = - \sum_p \int_{\Omega_p} \nabla S_i \cdot \sigma dV. \quad (8) \]

The stress over each particle domain is assumed to be approximately constant because particle domains are often small and variation of stress over them is negligible in comparison to variation of shape function gradients. In this case, the nodal internal forces can be calculated as

\[ f_{\text{int}}^i = - \sum_p \nabla \varphi_{ip} \cdot \sigma_p V_p, \quad (9) \]

in which \( \sigma_p \) is the stress over the \( p \)th particle domain, and

\[ \nabla \varphi_{ip} = \frac{1}{V_p} \int_{\Omega_x} \chi_p(x - x_p) \nabla S_i^*(x) dx. \quad (10) \]

At each time step, grid node accelerations, grid node velocities, particle velocities, and particle positions are calculated as follows:

\[ a_i = \frac{f_{\text{int}}^i + f_{\text{ext}}^i}{m_i} \quad (11) \]

\[ v_{i}^{n+1} = v_{i}^{n} + a_i \Delta t \quad (12) \]

\[ v_{p}^{n+1} = v_{p}^{n} + \sum_i \varphi_{ip} a_i \Delta t \quad (13) \]

\[ x_{p}^{n+1} = x_{p}^{n} + \sum_i \varphi_{ip} v_{i}^{n+1} \Delta t \quad (14) \]

The velocity gradient at particles is computed by

\[ \nabla v_{p}^{n+1} = \sum_i \nabla \varphi_{ip} v_{i}^{n+1} \]
Similarly, other kinematical quantities (such as the deformation gradient) are mapped to particles so that the particle stress tensor can be updated to the end of the time step by calling the constitutive model.

The conventional MPM considers each particle as a lumped mass, and there is no need to track particle domains in this method. For the GIMP method, two strategies are considered to track evolving particle domains under large deformations: uGIMP and cpGIMP. In the uGIMP, deformation of the particle domain is neglected and particle domains are tracked as fixed rectangles. In the cpGIMP, the particle sizes evolve based on only diagonal components of the deformation gradient at the particle so the particle domains remain rectangular. In the CPDI1 method, the updated particle domain at time step $n$ is determined using the fully updated deformation gradient as

$$r^n_1 = F^n p r^0_1$$
$$r^n_2 = F^n p r^0_2$$

where $(r^0_1, r^0_2)$ and $(r^n_1, r^n_2)$ are shown in Fig. 1. The following alternative grid shape functions are used in the CPDI method to efficiently calculate the integrals in Eq. (3) and Eq. (10) without incurring the expense of dividing the particle domains along cell boundaries:

$$S^*_i(x) = \sum_{\alpha=1}^{4} N_p^\alpha(x) S_i(x^\alpha_p) \quad \text{on} \quad \Omega_p.$$  \hspace{1cm} (17)

Here, $N^\alpha_p$ is the finite element shape function defined on the particle domain as a 4-node element. This shape function is defined for the $\alpha^{\text{th}}$ corner of the particle domain and $x^\alpha_p$ is the position of this corner. Using the alternative grid shape functions, Eq. (3) and Eq. (10) can be written as

$$\varphi_{ip} = \frac{1}{V_p} \int_{\Omega_p} S^*_i(x) dx = \frac{1}{V_p} \sum_{\alpha=1}^{4} \left( \int_{\Omega_p} N^\alpha_p(x) dx \right) S_i(x^\alpha_p)$$
$$= \frac{1}{4} \{ S_i(x^1_p) + S_i(x^2_p) + S_i(x^3_p) + S_i(x^4_p) \}$$  \hspace{1cm} (18)
\begin{align*}
\nabla \varphi_{ip} &= \frac{1}{V_p} \int_{\Omega_p} \nabla S_i^p(x) dx = \frac{1}{V_p} \sum_{\alpha = 1}^{4} \left( \int_{\Omega_p} \nabla N_{\alpha}^p(x) dx \right) S_i(x_\alpha^p) \\
&= \frac{1}{2V_p} \left\{ (S_i(x_1^p) - S_i(x_3^p)) \left[ r_{1y}^n - r_{2y}^n \right] + (S_i(x_2^p) - S_i(x_4^p)) \left[ r_{1x}^n + r_{2x}^n \right] \right\} \quad (19)
\end{align*}

Superiority of stability and accuracy of the CPDI1 solutions in comparison with the conventional MPM and GIMP solutions have been shown in [10].

3 THE CPDI2 METHOD

The original CPDI1 method tracks particle domains as parallelograms. The CPDI2 method, presented here, evolves particle domains as quadrilaterals. Specifically, particle domain corners are tracked instead of the particle centroid. When needed, the particle centroid \( x_p \) is determined based on the corner positions using the following equation:

\[ x_p = \frac{x_1^p + x_2^p + x_3^p + x_4^p}{4}, \quad (20) \]

where \( x_1^p, x_2^p, x_3^p, \) and \( x_4^p \) are positions of four corners of the domain of particle \( p \). The immediate conclusion is that there is no gap/overlapping between particle domains in the CPDI2 method. These particle domains are similar to a finite element mesh constructed using 4-node elements. Based on this algorithm, the particle domains are tracked as quadrilaterals. Similar to the CPDI1 formulation, using Eq. (17) as the alternative grid shape functions in the CPDI2 method, Eq. (3) and Eq. (10) can be written as

\begin{align*}
\varphi_{ip} &= \frac{1}{V_p} \int_{\Omega_p} S_i^p(x) dx = \frac{1}{V_p} \sum_{\alpha = 1}^{4} \left( \int_{\Omega_p} N_{\alpha}^p(x) dx \right) S_i(x_\alpha^p) \\
&= \frac{1}{4} \left\{ S_i(x_1^p) + S_i(x_2^p) + S_i(x_3^p) + S_i(x_4^p) \right\} \quad (21)
\end{align*}

\begin{align*}
\nabla \varphi_{ip} &= \frac{1}{V_p} \int_{\Omega_p} \nabla S_i^p(x) dx = \frac{1}{V_p} \sum_{\alpha = 1}^{4} \left( \int_{\Omega_p} \nabla N_{\alpha}^p(x) dx \right) S_i(x_\alpha^p) \\
&= \frac{1}{\beta_{1x}\beta_{2y} - \beta_{1y}\beta_{2x}} \left\{ S_i(x_1^p) \left[ -\beta_{2y} + \beta_{1y} \right] + S_i(x_2^p) \left[ \beta_{2y} + \beta_{1y} \right] \right. \\
&\left. + S_i(x_3^p) \left[ \beta_{2y} - \beta_{1y} \right] + S_i(x_4^p) \left[ -\beta_{2y} - \beta_{1y} \right] \right\} \quad (22)
\end{align*}

in which \( (\beta_{1x}, \beta_{1y}) \) and \( (\beta_{2x}, \beta_{2y}) \) are respectively the components of vectors \( \beta_1 = -x_1^p + x_2^p + x_3^p - x_4^p \) and \( \beta_2 = -x_1^p - x_2^p + x_3^p + x_4^p \).

A major advantage of the CPDI2 method in comparison with the conventional finite element method is that the CPDI2 method enforces no-slip contact between bodies automatically without any further computational costs.
4 ENRICHMENT FOR THE CPDI2 METHOD

As will be shown in the numerical simulations in the next section, spurious non-monotonic variation in stress can occur at material interfaces passing through the interior of a grid cell in the MPM techniques. This problem is caused by low-order shape functions being incapable of describing the jump in displacement gradients needed to allow the compliant materials within the cell to deform more than stiff materials. In this section, an enriched version of the CPDI2 method is presented to accurately model the material interfaces passing through the interior of a grid cell.

Conceptually, the CPDI2 begins an analysis step by mapping data from particles to the particle corners. This step is embedded in the final expression (Eq. (21)) which maps directly from particles to grid nodes to solve the equations of motion (EOMs) on the grid. Eq. (21) can be rewritten as

$$\varphi_{ip} = \frac{1}{V_p} \sum_{\alpha=1}^{4} \left( \int_{\Omega_p} N_{\alpha}^p(x) dx \right) S_i(x_{p,\alpha}^p) = \sum_{\alpha=1}^{4} R_p^\alpha S_i(x_{p,\alpha}^p)$$

(23)

in which

$$R_p^\alpha = \frac{1}{V_p} \int_{\Omega_p} N_{\alpha}^p(x) dx$$

(24)

In this equation, $R_p^\alpha$ can be interpreted as the mapping function between particle $p$ and particle corner $\alpha$, and $S_i(x_{p,\alpha}^p)$ can be considered as the mapping function between particle corner $\alpha$ and grid node $i$. If the algorithm were to map only to the corner nodes, then the resulting solution would be equivalent to an FEM solution. If the algorithm maps from corners to grid, then the resulting solution is the CPDI material point method. The particle domains in the CPDI2 are similar to 4-node finite element (Q4) with single point integration (particle corners and particles are analogous to FE nodes and Gauss points respectively).

To enrich the CPDI2 method, the nodal degrees of freedom already defined on the background grid can be supplemented with the corner values of the fields at the particles that are known to be near a material interface. This approach provides enrichment capable of properly describing weak discontinuities in the displacement field (i.e., strong discontinuities in strain) across a material interface that passes through the interior of a grid cell. Enriched CPDI2 is a hybrid of the two methods in which the MPM solution is used away from surfaces of discontinuity while the solution near the interface is resolved using the FEM solution that treats the corner nodes as supplemental degrees of freedom.

The distinguishing feature of enriched CPDI2 is that the grid nodes are supplemented with the enriched corner nodes for particles adjacent to an interface. As is done in all MPM formulations, the enriched CPDI2 algorithm loops over particles to accumulate contributions to the grid node mass, velocity, internal forces, etc., as in Eq. (1), Eq. (2), and Eq. (9). As is done in an ordinary CPDI2 implementation, the contribution of a particle to a grid node is evaluated as a sum of contributions from that particle’s corners.
In the loop over corners, non-enriched corners are treated the same as in a conventional CPDI formulation; namely,

\[ \varphi_{ip} = \sum_{\beta} R_{\beta}^p \zeta_{i\beta p} \]  

where

\[ \zeta_{i\beta p} = \begin{cases} S_i(x_\beta^p) & \text{if } \beta \text{ is not an enriched corner} \\ 1 & \text{otherwise} \end{cases} \]  

5 NUMERICAL EXAMPLES

In this section, effectiveness of the enriched CPDI2 method is verified using numerical examples. The following Neo-Hookean material model is used in all numerical simulations.

\[ \boldsymbol{\sigma} = \lambda \ln J \boldsymbol{I} + \mu \left( \boldsymbol{F} \boldsymbol{F}^T - \boldsymbol{I} \right) \]  

in which \( \boldsymbol{I} \) is the identity tensor, \( \mu \) and \( \lambda \) are the shear modulus and Lamé constant respectively, \( \boldsymbol{F} \) is the deformation gradient, and \( J \) is the determinant of \( \boldsymbol{F} \).

5.1 Vibration of a bi-material bar under self weight

Vibration of a vertical bar under its own weight is considered in this example. The upper end of the bar is fixed, the right and left boundaries have roller boundary conditions, and the lower end is traction free as shown in Fig. 2a. The bar is composed of two parts with different elastic moduli: \( E_1 = 2E_2 = 1 \times 10^7 \text{Pa} \). Poisson’s ratios and initial densities are \( \nu_1 = \nu_2 = 0.3 \) and \( \rho_1^0 = \rho_2^0 = 1050 \text{kg/m}^3 \), respectively. Time steps are chosen as \( \Delta t = 0.00005 \text{s} \). Gravity, \( g = -10 \text{m/s}^2 \), is applied suddenly as a step function at \( t = 0 \text{s} \). The initial problem domain is discretized by using 18 particles (2 per cell) as depicted in Fig. 2b. The material interface falls in the center of a grid cell.

Time histories of the displacement of particle A obtained from the GIMP, CPDI1, CPDI2, and enriched CPDI2 methods are presented in Fig. 3.
Figure 3: Time histories of the displacement of particle A in the bi-material bar under self weight simulations.

Figure 4: Time histories of the stresses of particles B and C in the bi-material bar under self weight simulations.

Without enrichment, a conventional MPM or CPDI solution to this problem exhibits a spuriously large stress in the stiff material and spuriously low stress in the compliant material. Fig. 4, which shows time histories of the stresses of particles B and C demonstrates that the enriched CPDI2 method improves the results by producing stresses at points B and C that are nearly equal to each other, as they should be. The stress profiles in Fig. 5 further illustrate the spurious non-monotonic variations in stress profiles near the material interfaces passing through the interior of a grid cell that are eliminated with enrichment.

5.2 Bi-material ring under centrifugal force

A bi-material ring under centrifugal force is simulated in this example. The ring is composed of two compliant and stiff rings as shown in Fig. 6. The following values are chosen for numerical simulations: modulus of elasticity $E_1 = 2E_2 = 1 \times 10^9$ Pa, Poisson’s ratios $\nu_1 = \nu_2 = 0.3$, initial densities $\rho_1^0 = \rho_2^0 = 1000 \text{kg/m}^3$, inner radius $r_i = 3 \text{m}$, outer radius $r_o = 3.2 \text{m}$, and time step $\Delta t = 0.000001 \text{s}$. Due to symmetry, only one-quarter of
the ring is modeled. The problem domain is discretized by using 1544 particles as shown in Fig. 6. The ring suddenly starts to rotate with a frequency of $\omega = 1\text{rad/s}$ at $t = 0$. To capture the centrifugal force, the following body forces (per unit mass) are applied to the numerical model:

$$b_r = \omega^2 r$$

$$b_\theta = 0$$

in which $b$ is the body forces in the cylindrical coordinates, $\rho$ is the density, and $r$ and $\theta$ are cylindrical coordinates.

Fig. 7 depicts time histories of the displacement of particle A (located as shown in Fig. 6), showing that CPDI2, enriched CPDI2, and FEM all give similar results for displacement.
Fig. 7: Time histories of the displacement of particle A in the bi-material ring under centrifugal force simulations.

Fig. 8: Time histories of the radial components of the stresses of particles B and C, respectively, in the bi-material ring under centrifugal force simulations.

Fig. 8 shows time histories of the radial components of the stresses of particles B and C. As shown in this figure, the CPDI2 method over predicts and under predicts stresses of particles B and C respectively. The enriched CPDI2 method leads to the similar stresses to the reference solution (i.e. the finite element solution).

6 CONCLUSIONS

An enhanced version of the convected particle domain interpolation (CPDI) method, named CPDI2, has been developed to further improve upon the accuracy of the original CPDI method by removing gaps/overlapping between particle domains without significantly impacting numerical efficiency. By modeling particle domains as quadrilaterals, the CPDI2 method not only offers greater flexibility in choosing particle domains shape in the initial configuration, but it also provides a natural computational framework for enrichment of fields through supplementing nodal degrees of freedom on the grid with the corner values of the fields at the particles near material interfaces. Accordingly, the
CPDI2 method has been demonstrated to be an efficient and accurate particle method in solving problems with weak discontinuities. As documented separately, the method also provides a natural means of enforcing boundary conditions. Future work will address strong discontinuities, such as fractures.

REFERENCES


ESTABLISHING CREDIBILITY OF PARTICLE METHODS
THROUGH VERIFICATION TESTING

Rebecca M Brannon†, Krishna Kanojji†a and Alireza Sadeghirad†

† Departments of Mechanical Engineering, University of Utah
70 S. Central Campus Dr., Salt Lake City, UT 84108, USA
email: rebeccabrannon@utah.edu, krishna.kanojji@gmail.com and
alirezasadeghirad@utah.edu

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Abstract. Within the particle methods community, standard benchmark tests are needed to demonstrate that the governing equations are solved correctly. Whereas the finite element method (FEM) has long-established basic verification standards (patch tests, convergence testing, etc.), no such standards have been universally adopted within the particle method community. As with FEM, particle methods must continue to pass patch tests, convergence, and frame basis indifference. Of greater contemporary value is the establishment of additional verification tests that exercise particle methods in massive-deformation problems involving complicated geometries, for which they purport to be superior to traditional finite-element methods. Two large-deformation verification problems, applicable to any constitutive model, are proposed to serve as standardized verification tests suitable to quantify accuracy, robustness, and convergence of particle methods. These new verification tests not only simultaneously confirm basis and frame indifference, but one of them also involves very large shear strains which are common in the application of the particle methods to penetration problems. One of these problems involves traction-free boundaries, which is the only boundary condition handled naturally in most particle methods. The other problem separately allows testing of boundary conditions.

1 Introduction

Verification and validation of codes with complicated numerical constitutive models is very important to establish confidence in the correctness and accuracy of these codes. Verification demonstrates that the governing equations are solved correctly in the code, whereas validation provides evidence that the equations themselves are realistic.

This paper defines two large-deformation problems, applicable to any constitutive model, that may serve as verification tests suitable to quantify accuracy, robustness, and convergence of particle methods. Both verification problems employ the method of
manufactured solutions (MMS) [1], which is an accepted standard [6, 7] for verification testing accomplished by running a simulation using the external body force field that has been analytically determined to achieve a pre-selected material motion.

The MMS approach has been extensively used in the fluid mechanics community [13], but is less frequently used in solid mechanics because of the mathematical complexity involved in deriving the analytical body force. A simple 1-D MMS for solids [8], which is constructed based on [6, 10], is already available as a familiarization exercise. Some straightforward 2-D examples may be found in [12].

The first part of this paper derives the analytical body force for the manufactured solution of a much more complicated generalized vortex deformation. Even though the displacement field for this problem is more complicated than other MMS problems in the literature, the nature of the local deformation is everywhere and at all times simple shear with superimposed rotation, thus making this problem a good candidate for general constitutive modeling since the model response must be determined analytically (or in tabular form) for only a single loading mode. This vortex problem involves traction free boundary conditions on either a circular or square domain, making the boundary conditions trivial to enforce in most particle methods. The error between the predicted material motion and the exact pre-calculated motion quantifies the error of the simulation. Numerical simulation results and spatial convergence studies are presented.

A second problem documented in detail separately [5], is similar to the generalized vortex problem in the sense that all points are subjected to identical loading modes (uniaxial strain with superimposed rotation), but includes the complication of nonzero traction on the boundary. The advantage of this MMS is that it checks the implementation of traction boundary conditions in the computational model. An even simpler preliminary test of traction boundary conditions, namely homogeneous deformation, is discussed in detail as a natural prerequisite exercise.

2 Generalized vortex problem

This section provides a detailed description of the MMS approach to deriving the analytical body force required to produce the pre-calculated material motion (simple shear with superimposed rotation), for what we refer to as the generalized vortex problem. The dynamic equation of motion is:

\[ \text{DIV}(\mathbf{T}) + \rho_s \mathbf{b} = \rho_s \mathbf{a} \] (1)

where \( \mathbf{a} \) is the acceleration, \( \mathbf{b} \) is the body force, \( \mathbf{T} \) is the first-Trelo Kirchhoff (FK1) stress, \( \rho_s \) is the initial density, and \( \text{DIV}(\mathbf{T}) \) is the backwards reference divergence of \( \mathbf{T} \), defined with respect to the Cartesian basis \((\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)\) by:

\[ \text{DIV}(\mathbf{T}) = \frac{\partial T_{ij}}{\partial X_j} \mathbf{E}_i = \frac{\partial \mathbf{T}}{\partial \mathbf{X}} : \mathbf{I} \] (2)

where \( "::" \) is the second-order tensor inner product, and \( \mathbf{I} \) is the second-order identity tensor. The problem domain is a ring of inner radius \( a \) and outer radius \( b \), as shown.
in Figure 1. The upcoming manufactured solution will have zero displacements and (to achieve traction-free boundaries) zero displacement gradients at the inner and outer radii. Thus, since material motion will occur only in the interior of the ring, this problem may be also regarded to apply on a square domain for which material outside the ring is prescribed to be stationary. This problem involves pure circular motion of all particles. The angular displacement varies with the radial coordinate, thus inducing simple shear with superimposed rotation at all times and at all spatial locations. For plane strain circular particle motion, the mapping from the initial position $X$ to the current position $x$ is given by

$$x = Q \cdot X.$$  \hfill (5)

Here, $Q$ is the orthogonal tensor with components

$$Q = \begin{bmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}$$  \hfill (1)

where $\alpha$ is the rotation angle, which varies with time and radial coordinate $R$ but not with angular coordinate $\Theta$. Specifically:

$$\alpha(R,t) = g(t)h(R)$$  \hfill (7)
where, $g(t)$ controls the amplitude of the deformation, and $h(R)$ controls relative radial variation of the rotation. The $h(R)$ function is selected in a way to ensure that material motion occurs only between the inner and outer radii, $a$ and $b$. Thus, $h(R) = 0$ for $R < a$ and $R > b$. For continuous displacements, this implies that $h(a) = h(b) = 0$. Moreover, choosing $h'(a) = h'(b) = 0$ ensures zero strain and hence zero traction at the boundary, which is typically easy to enforce in particle methods. The goal is to find the spatially varying body force field $b(R, \Theta)$ necessary to produce this motion.

To begin the analysis, the following lemmas are useful; for any scalar $s$,

$$\frac{dQ}{ds} = \frac{dQ}{d\alpha} \frac{d\alpha}{ds} = A \cdot \frac{dQ}{d\alpha}$$  \hspace{1cm} (6)

where $A$ is the axial tensor associated with the rotation axis. Namely:

$$A = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$  \hspace{1cm} (7)

The axial tensor has the important property that, for any vector $w$,

$$A \cdot w = E_z \times w$$  \hspace{1cm} (8)

where $E_z$ is the unit cylindrical base vector along the axis of rotation. Thus, for example, noting that the position vector is $X = R E_R$,

$$A \cdot X = E_z \times (R E_R) = R E_\Theta$$  \hspace{1cm} (9)

The following sections provide steps for determining the deformation gradient $F$, divergence of the PK1 stress $\text{DIV}(T)$, and acceleration $a$ required to ultimately solve (1) for the body force.

2.1 Deformation gradient and divergence of PK1 stress

Differentiating (7), the gradient of the rotation angle is given by

$$\frac{d\alpha}{dX} = g(t) \frac{dh}{dR} \frac{dR}{dX} = g(t) h'(R) E_R.$$  \hspace{1cm} (10)

The deformation gradient is found by taking the derivative of (3)

$$F = \frac{dX}{dX} = Q + X \cdot \frac{dQ^T}{d\alpha} \frac{d\alpha}{dX}. $$  \hspace{1cm} (11)

Using (6), (10), (9), and the fact that $Q^T \cdot A \cdot Q = A$, we have

$$F = Q \cdot (I + R g(t) h'(R) E_\Theta E_R).$$  \hspace{1cm} (12)
The terms in the parentheses represent a state of simple shear in the $\Theta$ direction with the shear plane tangent to the circumference. The multiplication by $Q$ represents additional superimposed rotation into the current configuration. Let

$$2\zeta(r) = Rh'(R).$$

Then the shear strain is given by

$$\epsilon(t, R) = g(t)\xi(R).$$

The deformation gradient in (12) may be written as

$$F = Q \cdot q \cdot \mathcal{F} \cdot q^T$$

where

$$\mathcal{F} = I + 2e(t, R)E_2E_1$$

and

$$q = \begin{bmatrix} \cos \Theta & -\sin \Theta & 0 \\ \sin \Theta & \cos \Theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$  

Note that

$$F = r \cdot \mathcal{F} \cdot q^T$$

where

$$r = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$  

Here, $\theta = \Theta + \alpha = \Theta + g(t)h(R)$, which is the angular coordinate of the particle in the deformed configuration. Note that $\mathcal{F}$ is an angle-independent “baseline” deformation representing simple shear without superimposed rotation. Further note that $\frac{d\mathcal{F}}{dR} = 2g(t)\xi'(R)E_2E_1$. Also, $q$ is independent of $R$, and $\frac{dq}{d\Theta} = A \cdot \mathbf{q}$. The tensor $r$ depends on the deformed angular coordinate, but (since the deformed angle varies with radial coordinate), this tensor implicitly depends on both angular and radial coordinates. Thus, applying the chain rule,

$$\frac{dr}{d\theta} = A \cdot r; \quad \left(\frac{\partial r}{\partial \Theta}\right)_R = A \cdot r; \quad \left(\frac{\partial r}{\partial R}\right)_\Theta = g(t)h'(R)A \cdot r$$

where subscripts are used to indicate what is held constant in partial derivatives. Let $S$ denote the second-Piola-Kirchhoff (PK2) stress associated with the deformation $\mathcal{F}$. Then, for an isotropic material, it follows that the PK2 stress $S$ associated with $F$ must be

$$S = q \cdot S \cdot q^T$$

The first Piola-Kirchhoff (PK1) stress associated with deformation $F$ is then

$$T = F \cdot S = Q \cdot q \cdot \tau \cdot q^T = r \cdot \tau \cdot q^T$$
where \( \tau = \mathcal{F} \cdot S \) is the \( \text{FKI} \) stress associated with the baseline deformation \( \mathcal{F} \), which depends on \( R \) indirectly through dependence of the shear strain on \( R \), but this baseline \( \text{FKI} \) stress is not dependent on the angular coordinate. Thus

\[
\left( \frac{\partial \tau}{\partial R} \right)_t = \frac{d\tau}{d\epsilon} \left( \frac{\partial \epsilon}{\partial R} \right)_t = \frac{d\tau}{d\epsilon} g(t) \xi'(R). \tag{21}
\]

The reference gradient of \( \text{FKI} \) stress is a third-order tensor given by

\[
\left( \frac{\partial T}{\partial X} \right)_t = \left( \frac{\partial T}{\partial R} \right)_{\Theta,t} E_R + \frac{1}{R} \left( \frac{\partial T}{\partial \Theta} \right)_{R,t} E_\Theta. \tag{22}
\]

Using (20), (18), and the chain rule, this equation becomes

\[
\left( \frac{\partial T}{\partial X} \right)_t = (g(t) \lambda'(R) A \cdot T + g(t) \xi'(R) r \cdot \frac{d\tau}{d\epsilon} \cdot q^T) E_R + \frac{1}{R} (A \cdot T + T \cdot A^T) E_\Theta. \tag{23}
\]

Referring to (2), recognizing that \( q^T \cdot E_R = E_1 \), and using (S) to note that \( A^T \cdot E_\Theta = E_R \), the reference divergence of \( \text{FKI} \) stress is given by

\[
\text{DIV}(T) = \rho_o (a - b) = g(t) \lambda'(R) A \cdot T \cdot E_R + g(t) \xi'(R) r \cdot \frac{d\tau}{d\epsilon} \cdot E_1
\]

\[+ \frac{1}{R} (A \cdot T \cdot E_\Theta + T \cdot E_R). \tag{24}\]

In terms of the deformed angular coordinate \( \theta \), the spatial cylindrical base vectors are

\[e_r = \cos(\theta) E_1 + \sin(\theta) E_2 \quad e_\theta = -\sin(\theta) E_1 + \cos(\theta) E_2. \tag{25}\]

Dotting (24) by these spatial cylindrical base vectors, the spatial cylindrical components of the divergence of \( \text{FKI} \) stress are given by

\[\rho_o (a_r - b_r) = (\xi'(R) \frac{d\tau_{11}}{d\epsilon} - h'(R) \tau_{21}) g(t) + \frac{1}{R} (\tau_{11} - \tau_{22}). \tag{26}\]

\[\rho_o (a_\theta - b_\theta) = (\xi'(R) \frac{d\tau_{21}}{d\epsilon} + h'(R) \tau_{11}) g(t) + \frac{1}{R} (\tau_{12} + \tau_{21}). \tag{27}\]

The key advantage of the above result is that it is expressed in terms of Cartesian components of the \( \text{FKI} \) stress corresponding to a baseline homogeneous pure shear, thus requiring the constitutive model to be evaluated only for that special case.

2.2 Velocity and acceleration

Using (3), (5), and (6), the velocity and acceleration of any given material particle are

\[v = \dot{Q} \cdot X = g'(t) h(R) A \cdot x = R \omega e_\theta, \tag{28}\]

\[a = g''(t) h(R) A \cdot x - (g'(t) h(R))^2 x = R \omega e_\theta - R \omega^2 e_r. \tag{29}\]

where

\[\omega = g'(t) h(R) \quad \text{and} \quad \dot{\omega} = g''(t) h(R). \tag{30}\]
2.3 Body force

The body force vector is given by

\[ \mathbf{b} = b_r \mathbf{e}_r + b_\theta \mathbf{e}_\theta. \]  

(31)

Using (26), (27), (29), and (30), the spatial cylindrical components of the body force are

\[ b_r = -R(g'(t)h(R))^2 - \frac{1}{\rho_o}((\xi[R] \frac{d\tau_{11}}{d\epsilon} - h'[R]\tau_{21})g(t) + \frac{1}{R}(\tau_{11} - \tau_{22})), \]  

(32)

\[ b_\theta = -R(g''(t)h(R)) - \frac{1}{\rho_o}((\xi[R] \frac{d\tau_{21}}{d\epsilon} + h'[R]\tau_{11})g(t) + \frac{1}{R}(\tau_{12} + \tau_{21})). \]  

(33)

The Cartesian components are obtained by substituting (25) into (31).

2.4 Numerical simulation

The above solution applies to any nonlinear elastic constitutive model. The constitutive model selected to illustrate the solution is the following simple Neo-Hookean model:

\[ \sigma = \frac{\lambda \log[J]}{J} \mathbf{I} + \frac{\mu}{J} \mathbf{F}^T \mathbf{F} - \mathbf{I} \]  

(31)

where, \( \lambda \) is the Lamé modulus, \( \mu \) is the shear modulus, \( J \) is the Jacobian of the deformation gradient \( \mathbf{F} \) and \( \mathbf{I} \) is the identity tensor. The initial density is chosen to be \( \rho_o = 100 \frac{\text{kg}}{\text{m}^3} \). Young’s modulus and Poisson’s ratio are chosen to be \( 10^8 \text{Pa} \) and 0.3 respectively (corresponding to \( \lambda = 577 \text{Pa} \) and \( \mu = 385 \text{Pa} \)). The inner and outer radii are 0.75 m and 1.25 m respectively. The final time of the simulation is \( T = 1 \text{s} \). The amplitude and distortion functions are taken to be \( g(t) = \sin(\frac{45}{100}t) \) and \( h(R) = (1 - 32(R - 1)^2 + 256(R - 1)^4) \). Based on these values the components of the body force are evaluated to be

\[ b_r = -\pi^2 R(15 - 32R + 16R^2)^4 \cos(\pi t)^2 + \frac{R\mu \sin(\pi t)^2(-64(R - 1) + 1024(R - 1)^3)^2}{\rho_o} \]  

(35a)

\[ b_\theta = -\frac{(64\mu(-45 + 188R - 240R^2 + 96R^3) + \rho_o \pi^2 R(15 - 32R + 16R^2)) \sin(\pi t)}{\rho_o} \]  

(35b)

This manufactured solution was implemented in the open-source Uintah MPM framework [11]. The results using two integration options (called uCDTR [4] and CTBD [2]) are presented. As seen in Figure 2, the simulation becomes unstable for uCDTR, but remains stable for CTBD. Even though the CTBD method gives superior results in comparison to all predecessor MPM methods, its final configuration shown in 3 still shows clear evidence of mesh and or particle distribution texture bias.
Figure 2: Deformed configurations for CTDI and uGMT near the peak rotation angle

Figure 4 shows convergence properties for this example using an $L_2$ error defined by

$$L_2\text{error} = \sqrt{\frac{\sum_{N_p} \| u_{\text{exact}}(x_p, t) - u_{\text{app}}(x_p, t) \|^2}{N_p}} \quad (36)$$

where $u_{\text{exact}}(x_p, t)$ and $u_{\text{app}}(x_p, t)$ are the analytical and calculated displacement vectors, respectively, and $N_p$ is total number of MPM particles. The top two plots in Figure 4 represent the time variation of error for four different mesh resolutions using CTDI and uGMT, respectively. The bottom two plots show standard rate of convergence plots of the error as a function of cell spacing at time $t = 1s$. The convergence plot for CTDI shows a normal decrease in error as the resolution is increased, with a rate of convergence close to 0.8. For the uGIMP method, on the other hand, the convergence plot lacks useful information because that method was unstable or crashed by time $t = 1s$ in all cases.

3 Homogeneous deformation

A 2-D homogeneous deformation MMS is illustrated here to check the implementation of traction boundary conditions in the simplest possible context. For a homogeneous deformation, the displacement field is given by

$$x = F \cdot X \quad (37)$$

where the deformation gradient tensor $F$ varies with time, but not position. To illustrate, we consider a deformation gradient that varies linearly in time according to $F = I(1 - t) + \mathcal{F}t$, where $\mathcal{F}$ characterizes the final deformed shape at the simulation step time of $t = 1s$. As the simplest possible example, the final deformation tensor for uniaxial strain, corresponding to a stretch $\lambda$ in the 1-direction is

$$\mathcal{F} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (38)$$
For homogeneous deformation of a homogeneous material, the gradient of stress is zero, implying, from (1), that the body force equals the acceleration. In this simple case of a linear morph of the deformation gradient from $I$ at time $t = 0$ to $\mathcal{F}$ at $t = 1$, the acceleration is zero, and hence the body force is zero. Boundary traction is given by $t = \sigma \cdot n$, where $\sigma$ is the Cauchy stress and $n$ is the unit outward normal. While a linearly morphing homogeneous deformation gradient has the advantage that the required body force is zero, the initial velocity field, $v = \dot{\mathbf{F}} \cdot \mathbf{X}$, is nonzero.

For illustration, the Neo-Hookean constitutive model in (34) will be applied to the uniaxial strain deformation in (35) using an initially square domain and peak stretch value of $A = 2$. The traction’s on the four faces of the domain are

$$t_1 = -t_2 = \left[ \frac{\lambda \ln(At - t + 1) + \mu((At - t + 1)^2 - 1)}{(At - t + 1)} \right] \mathbf{E}_1$$

$$t_3 = -t_4 = \left[ \frac{\lambda \ln(At - t + 1)}{(At - t + 1)} \right] \mathbf{E}_2$$

where $t_1$ is the traction on the positive $x$-face, $t_2$ is the traction on negative $x$-face, $t_3$ is the traction on positive $y$-face and $t_4$ is the traction on negative $y$-face. The initial problem domain is a unit square, discretized using $2 \times 2$, $4 \times 4$ and $8 \times 8$ grid resolutions with two particles per cell in each direction. Young’s modulus and Poisson’s ratio are $10^6$Ta and 0.25, respectively, with the stop time of the simulation $t = 1s$.

Figure 5 shows the deformation at various time steps. Again adopting the error definition in (36), the displacement field errors for the three resolutions are listed in table 1. It
Figure 4: Convergence plots for the stable CPEI simulations and unstable uGIMP simulations.

Table 1: $L_2$ error (meters) for various grid resolutions

<table>
<thead>
<tr>
<th></th>
<th>$2\times2$</th>
<th>$4\times4$</th>
<th>$8\times8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_2$</td>
<td>0.0733</td>
<td>0.0724</td>
<td>0.0724</td>
</tr>
</tbody>
</table>

can be seen that the problem has converged at $4\times4$ grid resolution. However, the failure to converge to machine precision indicates the need to investigate sources of error in the prescribed traction boundary condition algorithm for this code.

4 CONCLUSIONS

- Two large-deformation verification problems, applicable to any constitutive model (but illustrated using a simple elasticity model), were presented.

- The derivation of the analytical body force for a generalized vortex problem, which involved very large shear strains with traction free boundary conditions, was presented. Numerical simulation results with spatial convergence studies were provided for this problem.

- The method of manufactured solutions (MMS) for a simple homogeneous defor-
nition problem (uniaxial strain) was presented as a straightforward example of a
class of problems appropriate for assessing accuracy of traction boundary conditions,
which are notoriously difficult to implement in particle codes.

- These two verification problems were designed to have the same type of deformation
  (simple shear with superimposed rotation and uniaxial strain) at all material points.
  As such, these problems represent a rare case of being nontrivial MMS verification
  problems applicable to any - even highly nonlinear and history-dependent - constitutive
  model, provided that the response of the model to these standard loadings
  can be evaluated or tabulated.

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A MODIFIED STOKESIAN DYNAMICS METHOD FOR MINERAL SUSPENSIONS
ANDERS SAND*, MARTTI TOIVAKKA† AND JAN ROSENKRANZ**

* Division of Sustainable Process Engineering, Mineral Processing
  Luleå University of Technology
  971 87 Luleå, Sweden
  e-mail: anders.sand@ltu.se, www.ltu.se

† Laboratory of Paper Coating and Converting, and Centre for Functional Materials
  Abo Akademi University
  20500 Turku, Finland
  email: martti.toivakka@abo.fi, www.abo.fi

Key words: Stokesian dynamics, hydrodynamics, colloidal interactions, microstructure,
minerals, fine particles.

Abstract. A 3-dimensional modified Stokesian dynamics-based technique for simulating
mineral particle suspensions is presented. Stokesian dynamics is a mesh free particle
approach, which resembles the discrete element method. It includes hydrodynamic
interactions and other interparticle forces.

Expressions for the hydrodynamic interactions were modified based on results from finite
element (FE) calculation. The modifications allow for broader particle size distributions than
captured by traditional analytical expressions describing hydrodynamic interactions. In
addition, models are presented for colloidal interactions, steric repulsion caused by polymer
adsorbed onto mineral particles and the Brownian motion. These models expand the
applicability down to µm and nm size particles. Comparison between governing forces can be
made by generation of dimensionless expressions such as the particle Reynolds and Peclét
numbers.

Numerical simulations performed using this technique enable the study of microscopic
scale mechanisms and the characterisation of particle systems. This allows for appreciation of
microstructure development in time and the prediction of macroscopic level properties of
particle suspensions and consolidating systems.

This paper reports on both model development and results utilising the above-described
approach. In conclusion, the method is put into context by discussion of the applicability of
the method in various wet-state mineral processing applications.

1 INTRODUCTION

Particulate systems are of relevance in many industrial processes and products. To name
but a few, mineral processing, paper manufacturing, printing, paint production and many
biological and pharmaceutical applications are based on processing and handling of
particulate matter. Products can be in various forms, such as pellets, briquettes, powders or
tablets. Furthermore, during processing or as an end product, the material may exist in the form of a liquid suspension. This is exemplified by paint, paper coatings and printing inks.

Empirical studies of particle-based processes can in many cases be difficult or sometimes virtually impossible. This can be due to small size and time scales, intense external conditions (forces, pressures, temperatures, velocities) and complex particle interactions and system geometries. The understanding of liquid suspensions requires knowledge on both physical and chemical phenomena. It is often not possible to distinguish one effect from another, and therefore difficult to experimentally evaluate the relative influence of phenomena involved. In this respect, one can resort to numerical simulation for increasing ones understanding of the behaviour of materials in such processes. Simulation allows for adjustment of individual parameters and the possibility to explore the separate or combined influence of competing interaction models.

In mineral processing, particle simulation has traditionally been geared towards studies of dry-state granular material behaviour in complex geometries. Some examples include storage in silos, hopper discharge and conveyor transport processes [1]. Interparticle mechanical interactions and response to gravity and equipment behaviour (e.g. belt feeder translation) has in these cases often been sufficient in describing processes with relative accuracy. In more recent research, however, the focus has turned towards comminution and separation processes. In many cases, the models used for material transport simulation were simply transferred to the new fields of interest. To an extent it has been possible to gain improved understanding by this approach. There is a need, however, to improve models in terms of material property definitions and inclusion of more complex interactions and phenomena. There exist several examples of applications where such aspects which are now gaining relevance in mineral processing have been much more extensively studied. It is deemed possible to benefit from these interdisciplinary differences for improving simulation methodologies in mineral industry applications.

In a suspension, the behaviour of particles is governed by the macroscopic flow of liquid phase, hydrodynamic interparticle, particle-solid boundary and particle-free surface interactions. Colloidal interactions, the Brownian motion and various forces induced by the presence of polymers or other additives, are of relevance especially for nm to µm size particles. External field forces, as resulting from e.g. gravity and magnetic susceptibility of particles, can also play a significant role for the properties and behaviour of the suspension.

In this paper, the Stokesian dynamics method is introduced as an approach for simulating the behaviour of particles in suspension. Modifications to the original Stokesian dynamics approach are discussed. This includes adjustment of the hydrodynamic expressions in order to improve calculation accuracy for systems of broad particle size distribution and high solids concentration. Furthermore, models for various types of non-hydrodynamic interactions are presented. In a case study-type approach, the results of some studies utilising the models are discussed. Finally, areas of mineral processing are identified, where there could be benefits of using the Stokesian dynamics methods for increasing the understanding of particle-level phenomena and processes.
2 METHODOLOGY

Stokesian Dynamics is similar to Brownian Dynamics and the Discrete Element Method. DEM is typically applied on systems of a larger size scale than SD, which is strongly leaned towards liquid suspensions and colloidal-size interactions \cite{2}. Colloidal interactions are of importance for nm to µm size particles in suspension. One major difference is that Stokesian dynamics includes expressions for taking into account various types of hydrodynamic interactions \cite{3}. Furthermore, some type of coupling between the particles and liquid phase is needed to simulate flow in complex geometries. One approach is to import CFD/ FEM-generated flows to SD, and therefore obtain realistic liquid velocities and profiles \cite{4}. Although the suspending medium is typically assumed to be a Newtonian liquid, the combination of particles and liquid gives the suspension viscoelastic properties. The rheology will then be determined by the particle interaction models and parameters used. As indicated above, the method does not typically include back-coupling between the solid and liquid phases. Thus, macroscopic flow fields and interparticle liquid flow influence particles by forces and torques which induce translation and rotation on particles, but the particles themselves do not influence the flow of liquid. Full coupling can be obtained, but comes with added complexity and increased computational expense.

Stokesian dynamics is based on the N-body Langevin equation,

\[ m \frac{d \mathbf{U}(t)}{dt} = \mathbf{F}^H + \mathbf{F}^P + \mathbf{F}^B. \]  

which is simply a variant of Newton’s second law of motion. It states that the sum of all forces acting on a particle must balance with its mass and acceleration. The above forces are of different types. \( \mathbf{F}^H \) carries information on the hydrodynamic forces. These forces depend not only on particle positions but also on their velocities relative to each other and any externally applied flow field. \( \mathbf{F}^P \) are interparticle forces (e.g. colloidal, steric and other forces) which generally depend on interparticle distances and \( \mathbf{F}^B \) are stochastic single-particle forces e.g. as result of thermal vibration. If the particle Reynolds number is small, which is the case for small particles with low velocity difference relative to the continuous phase, an additional assumption can be made. In this event, the inertia of particles can be considered insignificant and the left side of equation (1) can be put as zero. This implies that the response of particles to the flow of surrounding liquid is instantaneous and that particles accelerate immediately to balance the force equation. Due to the complexity of interactions, SD-particles have with few exceptions been regarded as rigid spherical particles. There are examples, however, where ellipsoidal particles have been used. Ellipsoids are one of few cases of non-spherical particle shapes where exact mathematical expressions can be obtained for numerical calculation \cite{5}.

Below, models for hydrodynamic, colloidal and steric interactions are discussed. The effect of Brownian motion is included as a stochastic force. Additional interactions resulting from the presence of polymer in particle suspensions (bridging and depletion flocculation) are not considered in this work.
2.1 Hydrodynamic forces

In this chapter, the hydrodynamic forces are only briefly discussed. Further details on the hydrodynamic interactions have been presented by Nopola and Sand et al. \cite{4,6}.

Particle movement in a suspension is typically driven by the macroscopic flow of the liquid phase, often referred to as Stokes drag. Additional hydrodynamic interactions result from the movement of particles relative to each other, solid boundaries or to the free surface. One can separate between four different modes of particle relative motion; pumping, shearing, twisting and squeezing motion. A visualisation from the numerical simulations is shown in Figure 1.

The total net hydrodynamic force and torque on particles as result of the relative motions are calculated between each particle and nearby particles as given by the neighbour list.

Analytical expressions for the modes of relative motion has been presented by Kim and Karrila \cite{5}. These expressions, however, are only suitable for quite narrow particle size distributions. For particle size ratios beyond $\beta = 0.1$, an alternative approach needs to be used. Therefore, numerical simulations were performed based on finite element analysis and the results could be compared with the analytical expressions. The theoretical equations were then fitted with the numerical results in order to find better approximations of the forces and torques. A comparison between numerical results, analytical results by Kim and Karrila and modified expressions for the shearing relative motion is shown in Figure 2 \cite{4-6}.

![Figure 1. Squeezing relative motion as simulated and visualised using Elmer. Pressure (left) and liquid velocity vectors (right) \cite{6}.

Analytical expressions for the modes of relative motion has been presented by Kim and Karrila \cite{5}. These expressions, however, are only suitable for quite narrow particle size distributions. For particle size ratios beyond $\beta = 0.1$, an alternative approach needs to be used. Therefore, numerical simulations were performed based on finite element analysis and the results could be compared with the analytical expressions. The theoretical equations were then fitted with the numerical results in order to find better approximations of the forces and torques. A comparison between numerical results, analytical results by Kim and Karrila and modified expressions for the shearing relative motion is shown in Figure 2 \cite{4-6}.
In most cases good agreement between the analytical and numerical solutions was found. However, especially for large particle size differences and small interparticle surface separation distances, significant differences could be observed. Details on this procedure as well as the fitted equations are listed in Nopola and Sand et al. \[4,6\]. Furthermore, particle/solid boundary and particle/free surface interactions are described by Sand et al. \[6\].

### 2.2 Non-hydrodynamic forces

**Colloidal interactions**

The colloidal force between particles is a result of the conformation and distribution of ions and molecules of the suspending medium in response to the surface charge of particles. The colloidal interaction between two particles in a suspension has been formulated by the DLVO-theory (Derjaguin, Landay, Verwey, Overbeek) and is typically composed of an electrostatic repulsion and a van der Waals attraction component. The force between two charged particles can therefore be attractive or repulsive depending on the colloidal interaction parameters and the interparticle distance. The net colloidal interaction force is expressed as the sum of the electrostatic and van der Waals components

\[
F_{coll}^p = F_{el}^p + F_{vdw}^p.
\]

The electrostatic repulsive component is given by
\[ F_{el}^p = 4\pi \kappa \varepsilon_0 \varepsilon \psi_1 \psi_2 \frac{a_1 a_2}{a_1 + a_2} \frac{e^{-\kappa a}}{1 + e^{-\kappa a}} , \quad (3) \]

where \( \kappa \) is the reciprocal double layer thickness, \( \varepsilon \) the dielectric constant of the continuous phase, \( \varepsilon_0 \) the permittivity of vacuum, \( \psi_1 \) and \( \psi_2 \) the surface potentials of the interacting particles and \( \Delta \) the surface separation distance. \( a_1 \) and \( a_2 \) are the radii of the interacting particles \[7\]. The van der Waals attractive force can be described by

\[ F_{vdw}^p = -A_{vdw} \frac{\beta}{1 + \beta} \frac{\lambda (\lambda + 22.32\Delta)}{6\Delta^3 (\lambda + 11.116\Delta)^3} , \quad (4) \]

where \( A_{vdw} \) is the Hamaker constant, \( \lambda \) the London characteristic wavelength and \( \beta \) the size ratio between the larger and smaller particle \[7\].

**Steric repulsion**

Polymer dispersants are often added as a stabiliser to mineral suspensions. As polymer is adsorbed onto mineral particles they create a steric barrier which helps to increase interparticle distance and prevents agglomeration. The resulting steric force between particles is modelled as an osmotic pressure difference for surface separation distances less than twice the thickness of the adsorbed polymer layer. If the distance is less than the thickness of one polymer layer, an additional elastic force comes into play. This additional force is assumed to result from the compression of polymer chains, as the steric boundary layers overlap.

Thus, the steric force is described as

\[ F_{st}^p = F_{st, osm}^p + F_{st, el}^p , \quad (5) \]

The osmotic, \( F_{st, osm}^p \), and elastic, \( F_{st, el}^p \), components are calculated as

\[
F_{st, osm}^p = \begin{cases} 0 & \Delta \geq 2\delta_{st} \\ K_1 a (\Delta - 2\delta_{st}) & \delta_{st} < \Delta < 2\delta_{st} \\ K_1 a \left( \delta_{st} - \frac{2\delta_{st}^2}{\Delta} \right) & \Delta \leq \delta_{st} \end{cases} \quad (6)
\]

\[
F_{st, el}^p = \begin{cases} 0 & \Delta \geq \delta_{st} \\ K_2 a \delta_{st} \ln \left( \frac{4\delta_{st}^3}{\Delta (\Delta - 3\delta_{st})^2} \right) & \Delta < \delta_{st} \end{cases} \quad (7)
\]

where \( \Delta \) is the surface separation, \( \delta_{st} \) the polymer layer thickness, \( K_1 \) and \( K_2 \) are constants that depend on the effective volume fraction of polymer in the adsorbed layer and density,
molecular weight and solvency of the adsorbed polymer, and the other parameters as defined earlier [7].

**Brownian motion**

Brownian motion results from thermal vibration of particles and collisions with molecules of the suspending medium. The Brownian motion model is based on the Einstein equation for calculation of the mean Brownian displacement, $\bar{x}$, of a particle as function of time, $t$, as

$$\bar{x} = \sqrt{2Dt}.$$  \hspace{1cm} (8)

Particle diffusivity, $D$, is calculated as

$$D = \frac{RT}{6\pi\mu N_A},$$  \hspace{1cm} (9)

where $T$ is the system temperature, $\mu$ the viscosity of the continuous phase, $R$ the universal gas constant and $N_A$ Avogadro’s constant [7].

In this work, Brownian motion is produced by applying a force with random direction to each particle at every time step. The magnitude of the force is calculated with the help of an iteratively determined fitting parameter that takes into account system temperature and particle size range. The model showed good compliance with analytical results. More details on the model can be found in [6,8].

### 2.3 Analysis of Governing Forces

The interactions and forces described above can be evaluated in order to determine which models are relevant to include in simulations. This is done by forming ratios between forces, which will indicate which forces dominate over others. Values typical for the particle system and process under study should be used as parameters. This type of comparison can be very useful in understanding which models have the most influence on the process under investigation. Conversely, one can obtain indications whether some forces are insignificant and possible to exclude from the calculation. Common dimensionless numbers include the particle Reynolds and Peclét numbers [8].

The impact of hydrodynamic forces of the suspending medium on the particles can be described using the particle Reynolds number, $Re_p$. The particle Reynolds number can be calculated using the equation

$$Re_p = \frac{\rho_1 a_{char} u_{char}}{\mu},$$  \hspace{1cm} (10)

where $\rho_1$ is the density of the continuous (liquid) phase, $a_{char}$ the characteristic particle size, $u_{char}$ the characteristic velocity of the particles relative to the liquid and $\mu$ the viscosity of the suspension (Brady et al. 1988). In Stokesian Dynamics, the particle Reynolds number plays an important role due to the lubrication approximation, which assumes particles to react instantaneously to the flow of liquid. This approximation is valid for small particle Reynolds numbers.
The Peclét number, $Pe$, is used to compare the convective effect with the effect of particle diffusion. Convection is given by flow of the continuous phase, while diffusion results from Brownian motion. The Peclét number can be expressed as

$$Pe = \frac{6\pi a_{\text{char}} H u_{\text{char}}}{kT},$$

where $H$ is the characteristic length scale, $k$ the Boltzmann constant and $T$ temperature. The other parameters are as defined earlier. The characteristic length scale is chosen such that the movement of particles over this length scale would have significant effect on the microstructure or properties of the particle system.

A similar dimensionless expression can be established for comparing the relative influence of hydrodynamics in relation to colloidal interactions. The expression, here termed $Kc$, can be written as

$$Kc = \frac{a_{\text{char}} H u_{\text{char}}}{F_{el}^{P} + F_{vdw}^{P}},$$

where, $F_{el}^{P}$ is the electrostatic repulsion and $F_{vdw}^{P}$ the van der Waals attraction component of the DLVO interaction model.

What further complicates the use of these types of ratios is that conditions often change in dynamic simulation, both with geometry, particle size distribution and time. In such cases it is useful to establish intervals, to determine how the influence of various forces change with time or system properties.

3 SIMULATION RESULTS

In the following section we shortly review some studies making use of the modified Stokesian dynamics method, as described in this paper. In all cases, the properties of the particle systems are set to correspond to fine-grade mineral suspensions.

Filter cake properties

The structure of filter cakes as function of particle size, dewatering rate and temperature was studied [8]. The particle size range was 0.2 to 2 µm and a polydisperse system was also the subject of investigation. One can anticipate the filter cake structure to arise due to the ability or lack of ability of particles of each size and density fraction, to migrate against an absorption flow of liquid phase through a filter boundary. Assuming that only liquid is allowed to penetrate through the base substrate, the temperature and particle size-dependent Brownian motion will compete against the flow rate of the liquid. The solids profile in response to liquid flow rate, particle size, and temperature could be reported. Furthermore, size segregation effects could be studied for a polydisperse size distribution.

The mechanism of solids structure formation in the filtering process that takes place during paper coating consolidation has been a subject of dispute in the literature. One of the main results of this investigation was to show that both suggested mechanisms; thickening and filter cake formation, could occur. External conditions such as dewatering rate and
temperature will in combination with the properties of the suspension, determine which mechanism would dominate. It was also found that the concentration gradient noticed in thin filter cakes of polydisperse size distribution could be caused by a size segregation effect rather than the proposed thickening mechanism, Figure 3.

Figure 3. Size segregation in a filter cake composed of polydisperse particles at 3 different absorption rates. In this case, the filter cake is comprised of 1600 particles. Side view (above) and top view (below) [8].

A similar approach as presented in this work would be applicable for studies on, e.g., sedimentation rate depending on particle size and other system properties. It would also be possible to further the work on filtration processes and achieve a deepened understanding of prevalent mechanisms under various conditions and for various particle suspensions.

Colloidal interactions

DLVO-type colloidal interactions is considered to become significant if the size of particles is less than 10 µm. In many mineral processing applications such as comminution and particle separation processes, the particle size is often much larger and the consideration of these forces are not needed. However, the particle size distribution also needs to be taken into account. The small size fraction of a broad size distribution can fall under the colloidal size range, which in turn can influence the behaviour of the entire system [9]. One well known effect is a reduction of suspension viscosity as result of small particles acting as lubricants between larger particles.

In simulations there can be significant differences in particle behaviour, depending on if the colloidal forces are accounted for or not. For instance, Sand et al. [10] describes how the structure of consolidating calcium carbonate suspensions may be influenced by varying the colloidal interaction parameters. A typical effect is the formation of loose, rigid particle networks in systems dominated by van der Waals attraction. Conversely, repulsion dominated systems allow particles to arrange past each other and result in denser and less rigid particle networks. This behaviour is illustrated in Figure 4, where the consolidation of a fine-grade mineral suspension is simulated.
It was shown that even slight changes to DLVO-parameters can have influence on the solids concentration gradients and immobilisation times of suspensions and filter cakes. The accumulation of particles at the free surface of a mineral suspension during drying could to some extent be controlled by adjusting colloidal parameters\cite{8}.

The work illustrates the importance of understanding and controlling the colloidal properties of suspensions. A lack of understanding of these phenomena result in a number of process-related problems. Examples might include unwanted agglomeration, inhomogeneous distribution of additives, increased wear on equipment or abnormally high chemical consumption. These are factors which have not been extensively studied, except if necessitated by the constituents of the bulk.

**Suspension rheology**

The rheological behaviour of particle suspensions, or slurries, is complex. There can be variations in particle size, shape and concentration. The surface properties of particles and presence of additives will influence particle interactions and therefore also the macroscopic flow behaviour of the suspension. A suspension is typically non-Newtonian with rheological properties varying significantly with shear rate. The rheology of a suspension can be characterised empirically, but such investigations does not reveal the micro-level interparticle mechanisms that govern the behaviour of the particle-liquid system.

In this respect, particle dynamics simulation of slurry behaviour shows great promise. In the Stokesian dynamics approach presented in this work, suspension behaviour resulting from
hydrodynamic and colloidal interactions as well as adsorbed polymeric material can be investigated. The benefit of particle-level simulation, given proper model and parameter selection, is that most aspects related to the rheological properties of the slurry can come without preliminary assumptions regarding the slurry behaviour. This puts particle dynamics simulation in sharp contrast to continuum methods, where the rheological behaviour must be defined prior to simulation \[2\].

By Stokesian dynamics simulation of particles in shear and pressure-driven flows, it has been possible to report on rheology-related phenomena such as size segregation in polydisperse systems, lubrication effects by small particles in bimodal systems and dilatancy effects (structure jamming) in high solids concentration monodisperse systems \[4,11\]. The size segregation effect is illustrated in Figure 5.

![Figure 5. Example of size segregation in pressure-driven flow. Small particles preferentially migrate to the low shear rate region in the middle. Reproduced from \[7\].](image)

### 4 CONCLUDING REMARKS

This paper presents a simulation approach for investigating 3D particle motion in high solids concentration, low particle Reynolds number colloidal suspensions. The analytical expressions for the hydrodynamic interactions were modified by fitting to results from finite element analysis. This allows for simulation of broad size distributions. The method is thus applicable for a wide range of particle systems and colloidal-level phenomena. These include e.g. microstructure development in time, particle motion mechanisms, and macroscopic flow properties as result of the micromechanical behaviour of particles. The current model does not back-couple particle movement to the liquid flow field. This assumption is however acceptable if particles are moving at a velocity comparable to that of the suspending medium.

#### 4.1 Potential Applications of the Method in Mineral Processing

The modified Stokesian dynamics approach shows promise for simulation of high solids concentration fine particle solid-liquid systems, where particle interactions cannot be neglected. In addition, the validity of the Stokes law is assumed when describing the fluid’s drag forces, thus limiting the method to non-turbulent fluid flow. Considering these constraints, several potential applications of the Stokesian Dynamics method can be identified within the field of mineral processing. Here fine and ultrafine solid particles often occur as intermediates and as final products from ore beneficiation and industrial minerals production. They can also occur as unintended by-products and are in such cases frequently regarded as a disturbing factor. Possibly with some method or model adjustments, the areas where Stokesian Dynamics is expected to be of beneficial use can be grouped as follows:
**Slurry rheology**

The flow properties of mineral slurries are known to affect the operation of a variety of wet mineral processing equipment and are thus of relevance for optimal design and process control. This is obvious for flow-based separation processes where the slurry flow properties determine the outcome, as is the case in particle size separation and gravity separation. Analysing various types of equipment and their ordinary operating conditions indicates possible applications for sluices and spiral separators, but also for wet shaking tables in which thin film flow is used to concentrate the heavier particles \(^{12}\). Other suitable separation processes are jigging, where stratification of a particle bed by particle density is achieved via applying a pulsating fluid flow to loosen the bed of particles, and upstream classification or upstream sorting respectively using a continuous fluid flow instead. In all these cases Stokesian Dynamics could provide a useful tool to identify parameter settings for adjusting slurry density and viscosity in order to improve efficiency of mineral separation and throughput.

**Sedimentation and consolidation behaviour**

Dewatering is an important ancillary process in most mineral processing operations \(^{13}\). Knowledge of the settling properties of fine particle mineral slurries is required when designing efficient dewatering systems for mineral concentrates and tailings by means of thickening and filtration processes. Particle simulations based on Stokesian Dynamics allow studying fine particle slurry dewatering for different equipment geometries and process parameters. Using appropriate non-hydrodynamic interaction models, even the influence of flocculants can be systematically investigated, in order to improve dewatering efficiency and increase unit capacity.

**Particle agglomeration phenomena**

As with decreasing particle size the surface and contact forces become more dominant compared to the body forces, adhesion of fine particles to other particles or walls has to be considered in several unit operations for mineral processing. Studying particle agglomeration occurring within fine particle processing is therefore another area of application where Stokesian Dynamics based simulation can throw light upon the basic mechanisms of particle attachment and also detachment. This refers for instance to solids dispersion and mixing in the liquid phase, as well as the coating of grinding media and mill lining during comminution.

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MESHFREE LARGE DEFORMATION ANALYSIS WITH MODIFIED FORMULATION OF FLOATING STRESS-POINT INTEGRATION

YUKI ONISHI*, KENJI AMAYA*, and Ryuta IMAI†

* Department of Mechanical and Environmental Informatics, Tokyo Institute of Technology, Tokyo 152-8552, Japan
e-mail: yonishi@a.mei.titech.ac.jp, http://www.a.mei.titech.ac.jp/

† Mizuho Information & Research Institute, Inc., Tokyo 101-8443, Japan

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Abstract. A modified formulation of floating stress-point integration for large deformation analysis is presented. The modified formulation introduces an incremental internal force to the equilibrium equation instead of the virtual external force introduced in our previous formulation. With this modification, the temporal continuity of the mechanical equilibrium can be kept without introducing the virtual external force, and thus the accumulating error due to time advancing becomes small compared to our previous formulation. A few examples of large deformation analysis are also presented to show the validity and accuracy of the proposing method in comparison with the finite element method.

1 INTRODUCTION

Galerkin meshfree methods are expected to be effective numerical methods for solid mechanics problems that are difficult to be analyzed by finite element methods (FEM). One of such problems is large deformation problem that induces several hundred percent of strain[1]. Adaptive meshing techniques sometimes can help convergent capability of FEM, but are not widely used due to their complexity and imperfections. Accordingly, large deformation problems such as forming processes are competent application of meshfree methods.

Traditional Galerkin meshfree methods such as element-free Galerkin method (EFGM)[2] require background cells for integration over the analysis domain. The integration with background cells, however, has a difficulty in transportation of history-dependent states such as plastic strain, viscous strain, and total strain without numerical dispersion in
large deformation analysis. There are mainly two types of solution to the difficulty\[1\]:
nodal integration and stress-point integration. Nodal integration methods\[3, 4, 5, 6\] have
a common problem that numerical oscillation of zero-energy modes arises without artifi-
cial stabilization terms. Stress-point integration methods for large deformation problems
were studied by only a few\[7, 8, 9\], and the details of the formulation and quantitative
performance evaluation haven’t been shown so far.

We previously proposed a type of stress-point integration method named floating stress-
point integration\[11\] and presented its formulation and examples of analysis. The previous
formulation, however, has to introduce a virtual external force to enforce the temporal
continuity of the mechanical equilibrium. Being a cause of error increasing over time,
the virtual external force is problematic in terms of accuracy in highly large deformation
cases.

In this study, a modified formulation of floating stress-point integration is presented.
The modified formulation adopts the equilibrium equation in the incremental form in-
stead of the total form. With this modification, the temporal continuity of the mecha-
nical equilibrium can be kept without introducing the virtual external force, and thus the
accumulating error due to time advancing becomes small compared to our previous formu-
lation. In addition, the way of stress-point generation and support radius determination
are slightly modified. The detail of modified formulation of the proposing method and a
few examples of large deformation analysis are presented in this paper.

2 CONSTITUTIVE EQUATIONS

For the large deformation of isotropic elastic bodies, we adopt the following elastic
constitutive equations:

\[ T = C : E \quad \text{(i.e., } \dot{T} = C : \dot{D}) \],

where \( T \) is the Cauchy stress tensor, \( E \) is the Hencky strain tensor, \( \dot{T} \) is the Jaumann
rate of the Cauchy stress, \( \dot{D} \) is the stretching tensor, and \( C \) is the 4th order elasticity
tensor described as the following.

\[ C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + 2\mu \delta_{ik} \delta_{jl}, \]

where \( \lambda \) and \( \mu \) are the Lame’s parameters.

3 FORMULATIONS OF THE PROPOSING METHOD

For the sake of simplicity, we describe the proposing formulation for homogeneous ma-
terial under two-dimensional plane strain quasi-static condition. Note that the presenting
formulation can be easily extended to the formulation of heterogeneous material under
three-dimensional condition.

In this section, variables defined at a stress-point \( I \) are denoted with the superscript \( I \)
to the left of the variables. In a similar fashion, variables defined at a node \( J \) are denoted
with the subscript $J$ to the left of the variables. Also, trial variables of time increments are denoted with the superscript $+$ to the right of the variables.

The flowchart of the proposing method is shown in Fig.1 in advance. The following subsections in this section present the detail of each process of the flowchart.

### 3.1 Spacial Discretization and Initialization

Figure 2 shows the outline of the spacial discretization method in this study. The initial analysis domain is discretized into unstructured meshes with coarseness and fineness. The vertices defining the cells are treated as nodes, while stress-points are systematically generated in the cells and on the edges. Each stress-point $I$ holds its initial corresponding volume, $I^\text{ini}$, for the domain integration described later. Note that the cells and the edges are used only for the initialization of the nodes and stress-points and are never

![Flowchart of the proposing meshfree method. The detail of each process is described in §3.](image)

Figure 1: Flowchart of the proposing meshfree method. The detail of each process is described in §3.

![Outline of spacial discretization of the present method in two-dimensional cases. The cells are used only at the initial state and are never referred during the time advancing steps.](image)

Figure 2: Outline of spacial discretization of the present method in two-dimensional cases. The cells are used only at the initial state and are never referred during the time advancing steps.
referred during the time advancing steps.

In case of two-dimensional problems, the analysis domain is discretized into triangular meshes. Stress-points are generated at the center of each cell and at the center of each edge. The $V_{\text{ini}}$ are assigned as

$$V_{\text{ini}} = \begin{cases} \frac{1}{3}V_I & \text{(if } I \text{ is in a cell)} \\ \frac{1}{3}V_{IA} + \frac{1}{3}V_{IB} & \text{(if } I \text{ is on an edge)} \end{cases},$$

(3)

where $V_I$ is the volume of the cell including the stress-point $I$, $V_{IA}$ and $V_{IB}$ are the volumes of the cells pinching the stress-point $I$. The sum of $V_{\text{ini}}$ for all stress-points is equal to the volume of initial analysis domain.

The way of stress-point generation and corresponding volume distribution proposed here is not an optimal one but just an example. Optimization of the way is an issue in the future.

### 3.2 Shape Function and Its Derivatives

For the approximation of spacial variables, moving-least-square (MLS) approximation method[2] was employed. The polynomial basis used in this study is the 1st order polynomial basis given by

$$\{p(x)\} = \{1, x_1, x_2\},$$

(4)

where $x$ is the coordinates in the Cartesian space, $\{x_1, x_2\}^T$. For simplicity, the basis at a stress-point $I$ or a node $J$ are written as follows, respectively, later in this paper.

$$\{^Ip\} = \{p(Ix)\}, \quad \{^Jp\} = \{p(Jx)\}.$$

(5)

The weight function defined as a function of a positive parameter $d$, $w(d)$, is given by

$$w(d) = \begin{cases} \frac{1}{d} - 1 & (0 < d < 1) \\ 0 & (1 \leq d) \end{cases}.$$

(6)

The weight at a stress-point $I$ for a node $J$, $\{^Jw\}$, is defined as

$$\{^Jw\} = w\left(\|Jx - ^I \! Ix\|/^{IR}\right),$$

(7)

where $^{IR}$ is the support radius varied with time and the location of $I$. The way to decide $^{IR}$ is described later.

The shape function at a stress-point $I$, $\{^IN\} (= \{N(^I \! Ix)\})$, is given by

$$\{^IN\} = \{^Ip\} \left[^IA\right]^{-1} \left[^IB\right],$$

(8)
where \([I^A]\) and \([I^B]\) are matrices defined as
\[
[I^A] = \sum_{J \in \mathcal{I}} \{Jp\}^T \{Jp\},
\]
(9)
and
\[
[I^B] = \left[ \{Jw\} \{Jp\}^T, \{Jw\} \{Jp\}^T, \cdots, \{Jw\} \{Jp\}^T \right],
\]
(10)
where \(\mathcal{I}\) is the node set in the support domain of \(I\), \(J_k\) is the \(k\)th node member in \(\mathcal{I}\), and \(|\mathcal{I}|\) is the number of nodes in \(\mathcal{I}\).

The partial derivatives of the shape function with respect to \(I_{x_i}\), \(\{J'N\}'\), can be calculated as follows:
\[
\{J'N\}' = \left( \frac{\partial \{J'p\}}{\partial I_{x_i}} \right) [I^A]^{-1} [I^B] + \{Jp\} [I^A]^{-1} \left( \frac{\partial [I^B]}{\partial I_{x_i}} \right),
\]
(11)
where \(\frac{\partial [I^A]^{-1}}{\partial I_{x_i}}\) is a matrix given by
\[
\frac{\partial [I^A]^{-1}}{\partial I_{x_i}} = -[I^A]^{-1} \left( \frac{\partial [I^A]}{\partial I_{x_i}} \right) [I^A]^{-1}.
\]
(12)

From now, the value of the shape function at a stress-point \(I\) for a node \(J\) is written as \(\mathcal{I}N\). In addition, the vector consisting of spacial derivatives of \(\mathcal{I}N\) is written as \(\mathcal{I}N'\).

### 3.3 Integration Correction

For the satisfaction of integration constraints[4] or divergence-free condition[10], which is an essential qualification to pass the patch tests, integration correction should be applied. In this study, integration correction is realized by the scaling type correction[13]:
\[
\mathcal{I}N' = (1 + \lambda) \mathcal{I}N',
\]
(13)
where \(\mathcal{I}N'\) is the correction of \(\mathcal{I}N\) and \(\lambda\) is the correction coefficient independent from node \(J\). Equations of integration constraints in the proposing formulation are given by
\[
\sum_{\mathcal{I} \in \mathcal{J}} \mathcal{I}N' \mathcal{I}V = 0 \quad \text{(for \(\mathcal{I}\) in interior nodes)},
\]
(14)
\[
\sum_{\mathcal{I} \in \mathcal{J}} \mathcal{I}N' \mathcal{I}V - \mathcal{N} \mathcal{J}A = 0 \quad \text{(for \(\mathcal{I}\) in exterior nodes)},
\]
(15)
where \(\mathcal{J}\) is the set of stress-points such that have \(J\) in their support domain, \(\mathcal{N}\) is the nodal outward unit normal vector, and \(\mathcal{J}A\) is the nodal corresponding surface area. Substituting Eq.(13) into the Eqs.(14) and (15), we obtain the following simultaneous equation in the matrix form:
\[
[JN]\{\gamma\} = \{\mathcal{R}\},
\]
(16)
where $[\mathbf{N}']$ is the left-hand side matrix consisting of $f\mathbf{N}'$s, $\{\gamma\}$ is the left-hand side unknown vector consisting of $f\gamma$s, and $\{\mathcal{R}\}$ is right-hand side known vector consisting of residuals. Since the number of stress-points is greater than the number of nodes, Eq.(16) is an underdetermined system. In this study, we simply took the minimum norm solution as $\{\gamma\}$.

3.4 Quasi-implicit Time Advancing

Focusing on the highly large deformation analysis, the proposing method adopts the updated-Lagrangian approach. For the fully implicit time advancing with the updated-Lagrangian approach, update of the support, weight, and shape function of each stress-point is necessary in every convergent calculation of the backward difference. This update, however, causes difficulty of convergence.

We introduced a quasi-implicit time advancing scheme to overcome the difficulty of the fully implicit time advancing. In this scheme, variables to be updated are separated into two types, explicit variables and implicit variables, as follows.

3.4.1 Explicit Variables

The support radius, the weight, the shape function, and its derivatives for each stress-point are treated as explicit variables, which are updated before the starts of the Newton-Raphson loop in Fig.1. Thus these explicit variables are kept constant within each Newton-Raphson loop.

The support radius for a stress-point $I$, $^I\mathbf{R}$, is set to be a minimum value under the following required conditions:

- The number of nodes in the support is 6 or more ($|\mathcal{J}| \geq 6$),
- The condition number of $[^I\mathbf{A}]$ defined in Eq.(9) is less than $10^5$ (cond($[^I\mathbf{A}]$) < $10^5$).

In the actual implementation, $^I\mathbf{R}$ is initialized as a small value and multiplied by 1.01 iteratively until the conditions above are satisfied. This way to set $^I\mathbf{R}$ can avoid breakdowns of shape function construction in cases of non-uniform or irregular distribution of nodes. The other explicit variables are calculated as described in §3.2.

3.4.2 Implicit Variables

State variables of stress-points except the explicit variables are treated as implicit variables. The trial position of a stress-point $I$, $^I\mathbf{x}^+$, is updated by

$$ ^I\mathbf{x}^+ = ^I\mathbf{x} + \sum_{J \in \mathcal{J}} \int_J (\mathbf{N}'(J\mathbf{x}^+ - \mathbf{x})), $$

where $J\mathbf{x}^+$ is the trial position of a node $J$. The trial corresponding volume of a stress-point $I$, $^I\mathbf{V}^+$, is updated by

$$ ^I\mathbf{V}^+ = ^I\mathbf{V}^\text{ini} \cdot \det(^I\mathbf{F}^+), $$
where $^t\mathbf{F}^{+}$ is the trial total deformation gradient tensor. Other implicit variables of stress-points are calculated in the same fashion as the standard FEM[12].

### 3.5 Virtual Work Equation and Equilibrium Equation

One kind of form of the virtual work equation for solid mechanics[14] excluding the body force term is written as

$$
\int_v \tilde{\Pi}_t^T(t) : \delta \mathbf{F}_t(t) \, dv = \int_s \tilde{\mathbf{t}}_t(t) \cdot \delta \mathbf{u} \, ds,
$$

where $v$ is the current volume, $s$ is the current boundary, $\cdot$ denotes the material time derivatives, $\Pi_t(t)$ is the first Piola-Kirchhoff stress tensor in the current configuration, $\delta \mathbf{F}_t(t)$ is the variation of the deformation gradient tensor in the current configuration, $\tilde{\mathbf{t}}_t(t)$ is the surface traction vector in the current configuration, and $\delta \mathbf{u}$ is the variation of the displacement vector. Through the linear approximation of material time derivatives during an increment, $\delta \mathbf{F}_t(t)$ and $\mathbf{t}_t(t)$ can be approximated as $\Delta \Pi_t^{+}$ and $\Delta \mathbf{t}_t$, respectively.

By applying the Galerkin method to the proposed spatial discretization, $\delta \mathbf{u}$ and $\delta \mathbf{F}_t(t)$ can be discretized as $\{N\} \{\delta \mathbf{u}\}$ and $[\tilde{B}_N] \{\delta \mathbf{u}\}$, respectively, where $\{\delta \mathbf{u}\}$ is the variation of nodal displacement and $[\tilde{B}_N]$ is a matrix consisting of $\tilde{N}$'s. Consequently, the following discretized equilibrium equation in incremental form is obtained.

$$
\{\Delta \mathbf{f}^{\text{ext.}}\} + \{\Delta \mathbf{f}^{\text{int.}}\} = \{0\},
$$

where $\{\Delta \mathbf{f}^{\text{ext.}}\}$ is the nodal external force vector increment and $\{\Delta \mathbf{f}^{\text{int.}}\}$ is the nodal internal force vector increment given by

$$
\{\Delta \mathbf{f}^{\text{int.}}\} = \sum_{I \in \Omega} \int_{\Omega} [\tilde{B}_N]^T \{\Delta \Pi_t^{+}\} \, d\Omega \simeq \sum_{I \in \Omega} [\tilde{B}_N]^T \{\Delta \Pi_t^{+}\} \tilde{N}^{+},
$$

$$
[\tilde{B}_N] = \begin{bmatrix}
  d_{i|1} \tilde{N}_1 & 0 & \cdots & d_{i|1} \tilde{N}_1 & 0 \\
  0 & d_{i|2} \tilde{N}_2 & \cdots & 0 & d_{i|2} \tilde{N}_2 \\
  d_{i|2} \tilde{N}_2 & 0 & \cdots & d_{i|2} \tilde{N}_2 & 0 \\
  0 & d_{i|1} \tilde{N}_1 & \cdots & 0 & d_{i|1} \tilde{N}_1 
\end{bmatrix},
$$

$$
\Delta \Pi_t^{+} = \Delta \mathbf{t} - \mathbf{T} \left( (\mathbf{L}^+ \Delta t)^T - \text{tr}(\mathbf{L}^+ \Delta t) \mathbf{I} \right),
$$

where $\mathbf{L}$ and $\mathbf{I}$ are velocity gradient tensor and identity tensor, respectively. Since $\Delta \Pi_t^{+}$ approaches to $\mathbf{0}$ as $\Delta t$ approaches to $+0$, the left-hand side of Eq.(20) is also approaches to $\mathbf{0}$ as $\Delta t$ approaches to $+0$. Thus, Eq.(20) is always satisfied on the condition of $\Delta t = 0$ regardless of the update of the support before the start of the Newton-Raphson loop; the temporal continuity of the mechanical equilibrium between time increments is always achieved.

The way of stiffness equation construction and the way of boundary condition treatment are in the same fashion as standard FEM[12].
4 EXAMPLES OF ANALYSIS

For the accuracy verification of the proposing method, a few examples of analysis in plane strain condition are shown in this section. Commercial finite element software, ABAQUS/Standard[15], are used to make reference solutions.

4.1 Cantilever Bending Analysis

Figure 3 shows the initial analysis domain and locations of nodes and stress-points for the cantilever bending analysis. The domain is a 0.1 m × 1 m rectangular. The number of nodes, initializing cells, and stress-points are 335, 558, and 1450, respectively. The material of the domain is an elastic material of 1 GPa Young’s modulus and 0.3 Poisson’s ratio, i.e. $\lambda = 0.576923$ GPa and $\mu = 0.384615$ GPa. The left side nodes were geometrically constrained, and 400 kN concentrated force was applied to the top-right node toward the vertical downward direction. The analysis time span was discretized into 198 unequal time steps with automatic time step control. The solution of this problem using ABAQUS/Standard with 1000 ($=10 \times 100$) 2nd-order quadrilateral elements and 1000 equal time steps is prepared as a reference solution.

Figure 4 shows the deformed shape and Mises stress distribution in the final state. Figure 5 shows the relation between the applied vertical force and the vertical displacement at the top-right node. The displacement error of the proposing method is less than 0.3%. Though this analysis, it was confirmed that the proposing method can avoid the shear locking and has enough accuracy to solve large deflection analyses.

Figure 3: Initial locations of nodes (gray dots) and stress-points (blue dots) for the cantilever example.

Figure 4: Deformed shape and Mises stress distribution in the final state of the cantilever example with the proposing method (left) and ABAQUS/Standard (right).

Figure 5: Comparison of vertical displacement at the loading point (top-right corner node) of the cantilever example between the proposing method and ABAQUS/Standard.
4.2 Uniaxial Tension Analysis

Figure 6 shows the initial analysis domain and locations of nodes and stress-points for the uniaxial tension analysis. The domain is a 1 m × 1 m rectangular with a quarter circular hole of 0.8 m radius. The number of nodes, initializing cells, and stress-points are 873, 1,598, and 4,068, respectively. The material properties are the same as the previous example. The left side nodes were horizontally constrained; the bottom side nodes were vertically constrained; the top side nodes were horizontally constrained and displaced 1 m toward the vertical upward direction. The analysis time span was discretized into 352 unequal time steps with the automatic time step control. The solution of this problem using ABAQUS/Standard with 1,598 1st-order triangular elements meshed as the initializing cells and the automatic time step control is prepared as a reference solution.

Figure 7 shows the deformed shape and Mises stress distribution at the moment of 0.5 m displacement. Figure 8 shows the deformed shape and Mises stress distribution in the final

![Figure 6: Initial locations of nodes (gray dots) and stress-points (blue dots) for the uniaxial tension analysis.](image)

![Figure 7: Deformed shape and Mises stress distribution at the moment of 0.5 m displacement of the uniaxial tension analysis with the proposing method (left) and ABAQUS/Standard (right).](image)

![Figure 8: Deformed shape and Mises stress distribution at the moment of 1 m displacement of the uniaxial tension analysis with the proposing method.](image)

![Figure 9: Comparison of horizontal displacement at the bottom-right corner node of the uniaxial tension example between the proposing method and ABAQUS/Standard.](image)
state (1 m displacement) with the proposing method, while that with ABAQUS/Standard was not obtained because of excessive distortion and volumetric locking of elements. Figure 9 shows the relation between the enforced displacement and the horizontal displacement at the bottom-right node. As the displacement error of the proposing method is less than 1% until the limit of ABAQUS/Standard, the result of proposing method in the final state is expected to be appropriate.

4.3 Uniaxial Compression Analysis

Figure 10 shows the initial analysis domain and locations of nodes and stress-points for the uniaxial compression analysis. The domain is a 1 m × 0.5 m rectangular. The number of nodes, initializing cells, and stress-points are 528, 964, and 2,455, respectively. The material of the domain is an elastic material of 1 GPa Young’s modulus and 0.45 Poisson’s ratio, i.e. $\lambda = 3.103448$ GPa and $\mu = 0.3448276$ GPa. The left side nodes were horizontally constrained; the bottom side nodes were vertically constrained; the top side

Figure 10: Initial locations of nodes (gray dots) and stress-points (blue dots) for the uniaxial compression example.

Figure 11: Deformed shape and Mises stress distribution at the moment of 0.28 m displacement of the uniaxial compression example with the proposing method (left) and ABAQUS/Standard (right).

Figure 12: Deformed shape and Mises stress distribution at the moment of 0.4 m displacement of the uniaxial compression example with the proposing method.

Figure 13: Comparison of horizontal displacement at the bottom-right corner node of the uniaxial compression example between the proposing method and ABAQUS/Standard.
nodes were horizontally constrained and displaced 0.4 m toward the vertical downward direction. The analysis time span was discretized into 611 unequal time steps with the automatic time step control. The solution of this problem using ABAQUS/Standard with 964 1st-order triangular elements meshed as the initializing cells and the automatic time step control is prepared as a reference solution.

Figure 11 shows the deformed shape and Mises stress distribution at the moment of 0.28 m displacement. Figure 12 shows the deformed shape and Mises stress distribution in the final state (0.4 m displacement) with the proposing method, while that with ABAQUS/Standard was not obtained because of excessive distortion of elements. Figure 13 shows the relation between the enforced displacement and the horizontal displacement at the bottom-right node. The displacement error of the proposing method is less than 3% until the limit of ABAQUS/Standard. A few stress-points around the top-right corner, however, squeezed out of the analysis domain. Improvement of the update scheme of stress-point positions as prescribed in Eq.(18) is an issue to be resolved.

5 CONCLUSIONS

A modified formulation of floating stress-point integration for large deformation analysis was presented. The modified formulation based on the virtual work equation in the rate form introduces an incremental internal force to the equilibrium equation instead of the virtual external force introduced in our previous formulation. A scaling type integration correction was adopted so that the proposed method satisfied the divergence-free condition and passed patch tests. A quasi-implicit time advancing scheme was introduced to avoid both the convergence difficulty of the fully implicit scheme and the accumulating error of the fully explicit scheme.

Several examples of large deformation analysis were presented to show the validity and accuracy of the proposed method. The results of the proposed method agreed with those of ABAQUS/Standard within the range of ABAQUS/Standard gave the solution and seemed appropriate out of that range. Further improvements of stress-point arrangement and location update of stress-points will make the proposed method to be much stable and accurate. After these improvements, development of contact functions, and implementation of mixed formulations for nearly incompressible material etc., it would be expected that the proposed method could be an effective numerical method for practical large deformation analysis.

REFERENCES


MESHFREE METHOD FOR THE STOCHASTIC LANDAU-LIFSHITZ NAVIER-STOKES EQUATIONS

Anamika Pandey*, Axel Klar* ans Sudarshan Tiwari*

Fachbereich Mathematik
Technische Universität Kaiserslautern
Gottlieb-Daimler-Strasse, Gebäude 48,
Postfach 3049, 67653, Kaiserslautern, Germany
e-mail: pandey@mathematik.uni-kl.de, klar@mathematik.uni-kl.de,
tiwari@itwm.fhg.de

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Abstract. The current study aimed to develop a meshfree Lagrangian particle method for the Landau-Lifshitz Navier-Stokes (LLNS) equations. The LLNS equations incorporate thermal fluctuation into macroscopic hydrodynamics by addition of white noise fluxes whose magnitudes are set by a fluctuation-dissipation theorem. Moreover, the study focuses on capturing correct variance and correlation computed at equilibrium flows, which are compared with available theoretical values and found very good agreement.

1 INTRODUCTION

Physical quantities which describe a macroscopic system in equilibrium are seems to very near to their mean value. Nevertheless, due to microscopic fluctuation, random deviation from mean value though small, do occur. Thermal fluctuation is a source of noise in many system. Fluctuation plays a major role in phase transitions and chemical kinetics.

Investigation of thermal fluctuation in the motion of fluid becomes essential at micro and nano scale, because of the various applications of micro and nano scale flow, ranging from micro-engineering to molecular biology. Micro-machines have major impact on many disciplines (e.g. biology, medicine, optics, aerospace, and mechanical and electrical engineering) [1]. The study of fluctuation at micro and nano scale is particularly interesting when the fluid is under extreme conditions or near a hydrodynamic instability, e.g. the breakup of droplet in nanojet, fluid mixing in the Rayleigh-Taylor instability [8].

The validity of continuum approach has been identified with the validity of Navier-Stokes equations. This require the Knudsen number \( (Kn = \lambda / L) \) should be very small

\[ \lambda \text{ denotes mean free path and } L \text{ represents the characteristic length.} \]
compared with unity because the presence of thermal fluctuation becomes significant for larger Knudsen number \( (Kn \geq 0.01) \), which corresponds to rarefied regime, resulted in failure of continuum hypothesis \([2]\). Then the flow is computed with the help of kinetic equations. LLNS PDE which is an extended form of Navier-Stokes equation trying to capture the thermal fluctuation as accurate as possible.

To describe the general theory of fluctuation in fluid dynamics is equivalent to setting up the "equation of motion" for fluctuating quantities. Landau and Lifshitz has done this work by introducing the appropriate additional terms in the general equation of fluid dynamics and gave an extended form of Navier-Stokes equations. The Landau-Lifshitz Navier-Stokes equations is written by the expression

\[
U_t + \nabla \cdot F = \nabla \cdot D + \nabla \cdot S,
\]

where \( U \) stands for the vector of conserved quantities, density of mass, momentum and energy.

\[
U = \begin{pmatrix} \rho \\ J \\ E \end{pmatrix},
\]

\( F \) denotes the hyperbolic flux and \( D \) denotes the diffusive flux of fluid dynamics equations. \( F \) and \( D \) are given by

\[
F = \begin{pmatrix} \rho v \\ \rho v \cdot v + P I \\ v E + P v \end{pmatrix},
\]

\[
D = \begin{pmatrix} 0 \\ \tau \\ \tau \cdot v - q \end{pmatrix},
\]

where \( v \) is the fluid velocity, \( P \) is the pressure and \( T \) denotes the temperature. \( \tau = \eta \left( \nabla v + \nabla v^T - \frac{2}{3} I \nabla \cdot v \right) \) is the stress tensor. \( q = -\kappa \nabla T \) denotes the heat flux. Here \( \eta \) and \( \kappa \) are the coefficients of viscosity and thermal conductivity, respectively. For the given expression of \( \tau \) we have assumed the bulk viscosity is zero.

The given expression for \( \tau \) and \( q \) relates these quantities to the velocity and temperature gradients respectively. But, in the presence of fluctuation there are also spontaneous local stresses and heat fluxes in the fluid, which are not related to velocity and temperature gradient. For these spontaneous local stresses tensor and heat fluxes, the LLNS equations introduce additional vector in fluid dynamics equations called stochastic flux

\[
S = \begin{pmatrix} 0 \\ S \\ H + v \cdot S \end{pmatrix},
\]
where the stochastic stress tensor (SST) \( S \) and stochastic heat flux (SHF) \( H \) have zero mean and their covariances given by

\[
\text{Cov}(S_{ij}(r, t), S_{kl}(r', t')) = 2k_B\eta T \left( \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3} \delta_{ij}\delta_{kl} \right) \delta(r - r')\delta(t - t'),
\]

\[
\text{Cov}(H_i(r, t), H_j(r', t')) = 2k_B\kappa T^2 \delta_{ij}\delta(r - r')\delta(t - t'),
\]

\[
\text{Cov}(S_{ij}(r, t), H_k(r', t')) = 0.
\]

where \( k_B \) is the Boltzmann’s constant. These stochastic properties for \( S \) and \( H \) have been derived by a variety of approaches. Originally, these properties have been derived for equilibrium fluctuation [5, 9, 10, 11] and later validity of LLNS equations for non-equilibrium systems has been shown [12].

In this work a meshfree numerical scheme has been developed for solving LLNS equations. For simplicity, we will deal with one-dimensional system. We will solve Lagrangian form of LLNS. The Lagrangian form of LLNS for 1D system in terms of primitive variables can be written as

\[
\frac{D\rho}{Dt} = -\rho \frac{\partial u}{\partial x},
\]

\[
\rho \frac{Du}{Dt} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \frac{4}{3} \eta \frac{\partial u}{\partial x} \right) + \frac{\partial s}{\partial x},
\]

\[
c_v \rho \frac{DT}{Dt} = -P \frac{\partial u}{\partial x} + 4 \frac{\eta}{3} \left( \frac{\partial u}{\partial x} \right)^2 + \frac{\partial}{\partial x} \left( \kappa \frac{\partial T}{\partial x} \right) + s \frac{\partial s}{\partial x} + \frac{\partial h}{\partial x},
\]

\( u \) is the fluid velocity in x-direction and \( T \) is the temperature. \( s \) and \( h \) represent SST and SHF in 1D respectively. Momentum \( J = \rho u \) and energy density \( E = c_v \rho T + \frac{1}{2} \rho u^2 \) expressed in terms of \( \rho, u, T \). By \( D/Dt \) we denotes the Lagrangian derivative. We take the above system with equation of state \( P = \rho RT \), where \( R \) is gas constant.

We will demonstrate our result for a mono-atomic, hard sphere gas for which \( R = k_B/m \) and \( c_v = \frac{R}{\gamma - 1} \) where \( m \) is molecular mass and \( \gamma(= \frac{5}{3}) \) is the ratio of specific heat.

Now for covariances of stochastic fluxes in 1D system, from equations (6), (7) and (8)

\[
\text{Cov}(s(x, t), s(x', t')) = \frac{1}{\sigma^2} \int dy \int dy' \int dz \int dz' \text{Cov}(S_{xx}(r, t)S_{xx}(r', t')) = \frac{8k_B\eta T}{3\sigma} \delta(x - x')\delta(t - t').
\]

Similarly,

\[
\text{Cov}(h(x, t), h(x', t')) = \frac{1}{\sigma^2} \int dy \int dy' \int dz \int dz' \text{Cov}(H_x(r, t)H_x(r', t')) = \frac{2k_B\kappa T^2}{\sigma} \delta(x - x')\delta(t - t').
\]
here $\sigma$ represents the surface area of the system for $yz$-plane.

A number of numerical schemes have been developed for stochastic hydrodynamics equations. A stochastic lattice-Boltzmann model developed for simulating solid-fluid suspensions by Ladd [13]. In the following application of this approach for modelling Brownian motion of particles has been used by Sharma and Patankar [14], where they coupled the fluctuating hydrodynamics equations with the particle equations of motion which results in Brownian motion of particle.

Serrano and Español [15] have developed a thermodynamically consistent meanosscopic fluid particle model by casting their model into GENERIC structure which allows to introduce thermal fluctuation. They describe a finite volume Lagrangian discretization of the continuum equations of hydrodynamics using Voronoi tessellation.

Garcia et al. [3] has been developed a simple finite difference scheme for the linearized LLNS equations. This scheme was successful, but has been designed for specific problems and cannot extended in general due to certain assumption. In the context of Adaptive Mesh and Algorithm Refinement hybrid method that couple continuum and particle algorithms based on finite difference scheme has been developed. Demonstration of diffusion equation [18], the ”train model” [19] and the stochastic Burger’s equation [20] has been done by similar kind of scheme.

In the later work of Garcia et al. [4] CFD based scheme for stochastic PDE has been developed. In this work they have been considered compressible flow and developed numerical scheme for LLNS equations. Numerical schemes demonstrated equilibrium flow and computed spatial and time correlation at equilibrium result has been compared with theoretical value and DSMC simulation. Effect of fluctuation on shock drift has been shown and result compare with DSMC simulation. The most successful scheme has been considered in this work is ”Variance-preserving third order Runge-Kutta”. The method is based on a third order, TVD Runge-Kutta temporal integrator (RK3) combine with a centered discretization of hyperbolic and diffusive fluxes. This scheme has also incorporate a specific interpolation for required accuracy in variance.

In this work we will present a mesh free method for LLNS equations. We will consider Finite Pointset Method (FPM) like smoothed particle hydrodynamics (SPH) based on least square approach [16] for numerical solution of fluctuating hydrodynamics. We will concentrate here to capture correct variance in equilibrium flow and compare the result with theoretical values. The concluding section will emphasize on the successful mesh free simulation of fluctuating hydrodynamics equations for compressible flow and discuss future work. Since, it is a mesh free method and the distribution of particles (moving grid) can be quite arbitrary, the method is suitable for complicated geometry and multiphase flows. The FPM is suitable to handle a wide range of dynamical fluid structure interaction.

2 Numerical Method

The 1D Navier-Stokes equations have already solved with least square SPH like FPM for compressible flow [16]. A hybrid method also has been developed for kinetic and con-
tinum equations where the solution of kinetic equation has been done by DSMC and for continuum equations meshfree method used [17].

To extend the successful idea of meshfree method for 1D Navier-Stokes equations we will solve 1D LLNS equations with a meshfree Lagrangian method. Though, it is a bit difficult to develop a meshfree framework for stochastic partial differential equations (SPDE) due to already existed randomization in position of mesh particles, it has a number of advantage likewise the meshfree method is a more natural choice to study the dynamics of small particles at fluid interfaces, to generate a hybrid method for coupling of Boltzmann and fluctuating hydrodynamics equations for very small geometry. Earlier studies deal the coupling of DSMC for Boltzmann equation and finite volume method for the LLNS [21].

In this method the particle position are itself the grid and to take this consideration in account we will simulate an additional equation with (9 - 11). This equation will determine the particle position and given as

\[ \frac{Dx}{Dt} = u. \]  

(14)

Here \( u \) is the fluid velocity and \( x \) denote the position of particle in 1D. To approximate spatial derivative at every grid point is equivalent to approximate the spatial derivative at every particle positions. For solving the Lagrangian LLNS system given by (9-11) together with (14) by FPM, first we fill the domain by particles. These particle moves with fluid velocity and then approximate spatial derivative in equation (9-11) at each particle position from its neighbouring particles. This reduce the given system of partial differential equations (PDE) to a system of ordinary differential equations (ODE) with respect to time per particle.

We will use MacCormack scheme [4] for reduced ODE on each particle. This MacCormack scheme is a variant of Lax-Wendroff. On applying the desired MacCormack’s discretization of LLNS will be

**Step 1**

\[ x_i^* = x_i^n + \Delta t u_i^n, \]  

(15)

\[ \rho_i^* = \rho_i^n - \Delta t \rho_i^n \left( \frac{\partial u}{\partial x} \right)_i^n, \]  

(16)

\[ u_i^* = u_i^n + \frac{\Delta t}{\rho_i^n} \left\{ - \left( \frac{\partial P}{\partial x} \right)_i^n + \frac{4}{3} \frac{\eta_i^n}{\rho_i^n} \left( \frac{\partial^2 u}{\partial x^2} \right)_i^n + \frac{4}{3} \frac{\partial u}{\partial x} \left( \frac{\partial u}{\partial x} \right)_i^n + \left( \frac{\partial s}{\partial x} \right)_i^n \right\}, \]  

(17)

\[ T_i^* = T_i^n + \frac{\Delta t}{c_v \rho_i^n} \left\{ - P_i^n \left( \frac{\partial u}{\partial x} \right)_i^n + \frac{4}{3} \frac{\eta_i^n}{\rho_i^n} \left( \frac{\partial u}{\partial x} \right)_i^n \right\} + s_i^n \left( \frac{\partial u}{\partial x} \right)_i^n + \frac{\partial h}{\partial x} \left( \frac{\partial T}{\partial x} \right)_i^n \]  

+ \left( \frac{\partial \kappa}{\partial x} \right)_i^n \left( \frac{\partial T}{\partial x} \right)_i^n, \]  

(18)
Step 2

\[ x_{i}^{**} = x_{i}^{*} + \Delta tu_{i}^{*}, \]
\[ \rho_{i}^{**} = \rho_{i}^{*} - \Delta t \rho_{i}^{*} \left( \frac{\partial u}{\partial x} \right)_{i}^{*}, \]
\[ u_{i}^{**} = u_{i}^{*} + \frac{\Delta t}{\rho_{i}^{*}} \left\{ - \left( \frac{\partial P}{\partial x} \right)_{i}^{*} + \frac{4}{3} \eta_{i}^{*} \left( \frac{\partial^{2} u}{\partial x^{2}} \right)_{i}^{*} + \frac{4}{3} \left( \frac{\partial \eta}{\partial x} \right)_{i}^{*} \left( \frac{\partial u}{\partial x} \right)_{i}^{*} + \left( \frac{\partial s}{\partial x} \right)_{i}^{*} \right\}, \]
\[ T_{i}^{**} = T_{i}^{*} + \frac{\Delta t}{c_{v} \rho_{i}^{*}} \left\{ - P_{i}^{*} \left( \frac{\partial u}{\partial x} \right)_{i}^{*} + \frac{4}{3} \eta_{i}^{*} \left( \left( \frac{\partial u}{\partial x} \right)_{i}^{*} \right)^{2} \right\} + \kappa_{i}^{*} \left( \frac{\partial^{2} T}{\partial x^{2}} \right)_{i}^{*} \]
\[ + \left( \frac{\partial \kappa}{\partial x} \right)_{i}^{*} \left( \frac{\partial T}{\partial x} \right)_{i}^{*} + s_{i}^{*} \left( \frac{\partial u}{\partial x} \right)_{i}^{*} + \left( \frac{\partial h}{\partial x} \right)_{i}^{*} \right\}, \]

Final Step

\[ x_{i}^{n+1} = \frac{1}{2} \left( x_{i}^{n} + x_{i}^{**} \right), \]
\[ \rho_{i}^{n+1} = \frac{1}{2} \left( \rho_{i}^{n} + \rho_{i}^{**} \right), \]
\[ u_{i}^{n+1} = \frac{1}{2} \left( u_{i}^{n} + u_{i}^{**} \right), \]
\[ T_{i}^{n+1} = \frac{1}{2} \left( T_{i}^{n} + T_{i}^{**} \right), \]

For each step given above \( P, \eta, \kappa \) will be computed by

\[ P = \rho RT, \]
\[ \eta = \frac{5}{16d^{2}} \sqrt{\frac{mk_{B}}{\pi} T}, \]
\[ \kappa = \frac{15k_{B}\eta}{4m}, \]

Here \( d \) denotes the molecular diameter. \( n = 0, 1, 2, \ldots \) represents the time step and \( i = 1, 2, \ldots N \) goes for particles in domain.

The approximation for SST and SHF for each particle at any instant is computed as

\[ s_{i}^{n} = \sqrt{\frac{8k_{B}}{3\Delta t V_{c}} \left( \eta_{i}^{n} T_{i}^{n} \right) \Re_{i}^{n}}, \]
\[ \kappa_{i}^{n} = \sqrt{\frac{2k_{B}}{\Delta t V_{c}} \left( \kappa_{i}^{n} (T_{i}^{n})^{2} \right) \Re_{i}^{n}}, \]
where $V_c$ denotes the volume between two particle of spatial discretization and $\mathcal{R}$ are independent, identically distributed (iid), Gaussian random value with zero mean and unit variance.

The stochastic fluxes required some extra care in two-step scheme. The $s$ and $h$ are independent, identically distributed (iid) Gaussian random variable with mean zero and variance $\sigma^2$ for $l = n, \ast$. Let denotes $s$ and $h$ in combined by $s$. Substituting this in MacCormack scheme we find variance in the stochastic flux $s$ on simulation particle as

$$\text{Var} \left( \left( \frac{1}{2} s^n + \frac{1}{2} s^\ast \right)^2 \right) = \left( \frac{1}{2} \right)^2 \text{Var} (s^n) + \left( \frac{1}{2} \right)^2 \text{Var} (s^\ast)$$

$$= \frac{1}{2} \text{Var} (s)$$

$$= \frac{\sigma^2}{2}.$$  \hspace{1cm} (32)

We have neglected the multiplicity of noise by taking $\text{Var} (s^n) = \text{Var} (s^\ast)$.

The above equation means that because of the temporal averaging variance in the flux reduced to half of its original magnitude. So, to include this observation the correct stochastic flux for a two step scheme will be $\tilde{s} = \sqrt{2} s$ instead of $s$.

Now we have to solve the equations (15 - 29) and for this the remaining task is to approximate the spatial derivatives on right hand side of the prescribed equations.

### 2.1 Meshfree approximation of spatial derivatives

In many practical applications the mesh plays a very important role in simulation and many solvers loose their accuracy if the mesh is poorly constructed. In some complicated geometry the mesh generation becomes a difficult task. A meshfree method does not require a regular grid and gives a very good approximation of spatial derivative even for randomly distributed grid point so overcome to mesh generation difficulties. Initially we will fill the domain with particles in a regular grid method but when they move with fluid velocity then their distribution become quite arbitrary after short time.

We will describe the least square approximation of spatial derivatives in 1D. As mentioned earlier, in this method grid points are particle positions. Therefore, we have to approximate the derivative at every particle position. Let $f(t, x)$ be a scalar function at $x$ and $f_i(t)$ its value at $x_i \in [0, L]$ for $i = 1, 2, 3, \ldots, N$ for any instant $t$. Approximation of spatial derivatives of $f(x)$ at $x$ will be in terms of the values of $f(x)$ on a set of neighbouring points. For limiting number of neighbouring points of $x$ we will consider a weight function $w = w(x_i - x; h)$ with small compact support, where $h$ determines the size of support. The choice of weight function can be quite arbitrary but we will consider
a Gaussian weight function in the following form

\[
w(x_i - x; h) = \begin{cases} 
\exp \left( -\alpha \frac{\|x_i - x\|^2}{h^2} \right), & \text{if} \quad \frac{\|x_i - x\|}{h} \leq 1 \\
0, & \text{else.}
\end{cases}
\]  

with \(\alpha\) a positive constant, we have taken the value of \(\alpha\) is 6.25, \(h\) defines the neighbourhood radius for \(x\). Let \(P(x, h) = \{x_i : i = 1, 2, \ldots, n_x\}\) be the set of \(n_x\) neighbouring points of \(x\) in an interval of radius \(h\). For consistency reason some obvious restriction required for \(h\) as there should be enough number of neighbouring particle for least square approximation. In general for 1D, \(h = 3dx\), where \(dx\) is the initial spacing of particles.

Derivatives of function can be computed easily and accurately by using Taylor’s series expansion and the least square approximation. We will write Taylor’s series expansion of \(f(t, x)\) around \(x\) with unknown coefficients and then compute these coefficients by minimizing the error over the neighbouring points.

Suppose we want to approximate the derivatives of a function \(f(t, x)\) from its \(n_x\) neighbouring points sorted with respect to its distance from \(x\). Consider Taylor’s expansion of \(f(t, x_i)\) around \(x\)

\[
f(t, x_i) = f(t, x) + (f(t, x))_x (x_i - x) + \frac{1}{2} (f(t, x))_{xx} (x_i - x)^2 + e_i
\]

where \(e_i\) is the error in Taylor’s expansion at the point \(x_i\). The unknowns \(f_x, f_{xx}\) are required derivatives computed by minimizing the error \(e_i\) for \(i = 1, 2, 3, \ldots, n_x\). The above system can be written as

\[
\vec{e} = M\vec{a} - \vec{b}
\]

where,

\[
M = \begin{pmatrix}
x_1 - x & \frac{1}{2} (x_1 - x)^2 \\
x_2 - x & \frac{1}{2} (x_2 - x)^2 \\
\vdots & \vdots \\
x_{n_x} - x & \frac{1}{2} (x_{n_x} - x)^2
\end{pmatrix}
\]

\(a = [f_x, f_{xx}]^T\), \(b = [f_1 - f, f_2 - f, \ldots, f_{n_x} - f]^T\) and \(e = [e_1, e_2, e_3, \ldots, e_{n_x}]^T\).

For \(n_x > 2\) this system will be over-determined for two unknowns \(f_x\) and \(f_{xx}\). The unknowns \(\vec{a}\) are obtained from a weighted least square method by minimizing the quadratic form

\[
J = \sum_{i=1}^{n_x} w_i e_i^2 = (M\vec{a} - \vec{b})^T W (M\vec{a} - \vec{b})
\]

(37)
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where

\[
W = \begin{pmatrix}
  w_1 & 0 & \ldots & 0 \\
  0 & w_2 & \ldots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \ldots & w_n \\
\end{pmatrix}
\]

Finally, the minimization of \( J \) gives

\[
\vec{a} = (M^T W M)^{-1} (M^T W) \vec{b}
\]

required derivatives of function \( f(t, x) \) as a linear combination of discrete neighbour values \( f_i \).

3 Numerical Results

3.1 Equilibrium

This section gives results of described method for equilibrium scenario. The physical domain has been chosen such that the fluctuation in system becomes significant. System’s parameter for numerical simulation are given in Table 1.

<table>
<thead>
<tr>
<th>System parameter in CGS units for simulation of dilute gas.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular diameter (Argon) 3.66 × 10^{-8}</td>
</tr>
<tr>
<td>Reference mass density 1.78 × 10^{-3}</td>
</tr>
<tr>
<td>Sound speed 30781</td>
</tr>
<tr>
<td>System length 1.25 × 10^{-4}</td>
</tr>
<tr>
<td>System volume 1.96 × 10^{-16}</td>
</tr>
</tbody>
</table>

The initial spacing of particle will be \( dx = L/N \), where \( N \) is the initially distributed particles in domain. Initially 40 number of particles has been considered in domain. This number will not fixed during simulation and there will be an updating in number of particles.

The stability condition is found to be consistent with that suggested in [4].

\[
(| u | + c_s) \frac{\Delta t}{\Delta x} \leq 1
\]

\[
\max \left( \frac{4 \bar{\eta}}{3 \bar{\rho}} \frac{\bar{\kappa}}{\bar{\rho} c_v \Delta x^2} \right) \leq \frac{1}{2}
\]

where \( c_s \) is the sound speed; the bar indicates the reference value of quantities around which system fluctuate. For the given reference state in Table 1 and initial spacing of particle, the time step has been chosen \( \Delta t = 10^{-13} \text{s} \).
3.2 Variance at Equilibrium

The first benchmark for given schemes is capturing correct variance of conserved variables for a system at equilibrium. For test problems, we consider a periodic domain with zero net flow and constant non-zero net flow. We take constant average density and temperature in both cases as given in Table 1. The variance computed from $10^7$ samples. Due to moving grid we will calculate statistics in global sense as given below

$$mean (\rho) = E(\rho) = \frac{1}{\sum_{n=1}^{N_s} M(n)} \left( \sum_{n=1}^{N_s} \sum_{i=1}^{M(n)} \rho_i^n \right),$$  

(41)

$$Var (\rho) = E(\rho^2) - (E(\rho))^2$$

$$= \frac{1}{\sum_{n=1}^{N_s} M(n)} \left( \sum_{n=1}^{N_s} \sum_{i=1}^{M(n)} (\rho_i^n)^2 \right)$$

$$- \left( \frac{1}{\sum_{n=1}^{N_s} M(n)} \left( \sum_{n=1}^{N_s} \sum_{i=1}^{M(n)} \rho_i^n \right) \right)^2,$$  

(42)

Here, $N_s$ is the total number of samples and $M(n)$ is the number for particle at time $(nSkip + n)\Delta t$ ($nSkip$ is the number of initial time step for stabilizing the system). In the same way statistics for momentum and energy can be computed.

Tables 2 and 3 compare the theoretical variances have been computed in ([6], [3]) with measured variances in meshfree stochastic scheme.

<table>
<thead>
<tr>
<th>Variance of</th>
<th>Exact value</th>
<th>Meshfree MacCormack</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (\rho)</td>
<td>$2.35 \times 10^{-8}$</td>
<td>$2.11 \times 10^{-8}$</td>
<td>$-10.2%$</td>
</tr>
<tr>
<td>Momentum (\textbf{J})</td>
<td>13.34</td>
<td>13.33</td>
<td>$-0.07%$</td>
</tr>
<tr>
<td>Energy (\textbf{E})</td>
<td>$2.84 \times 10^{10}$</td>
<td>$2.68 \times 10^{10}$</td>
<td>$-5.6%$</td>
</tr>
</tbody>
</table>
Table 3: Variance in conserved quantities at equilibrium for constant non-zero net flow.

<table>
<thead>
<tr>
<th>Variance of</th>
<th>Exact value</th>
<th>Meshfree MacCormack</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density ($\rho$)</td>
<td>$2.35 \times 10^{-8}$</td>
<td>$2.12 \times 10^{-5}$</td>
<td>$-9.7%$</td>
</tr>
<tr>
<td>Momentum ($J$)</td>
<td>$18.91$</td>
<td>$19.01$</td>
<td>$+0.05%$</td>
</tr>
<tr>
<td>Energy ($E$)</td>
<td>$3.67 \times 10^{10}$</td>
<td>$3.85 \times 10^{10}$</td>
<td>$+4.9%$</td>
</tr>
</tbody>
</table>

4 Conclusion

Stochastic Partial differential equation were discussed for modelling fluctuation in compressible flow of gas dynamics. For numerical simulation of the SPDEs a meshfree discretization approach has been introduced. The results of the simulation shows that the Lagrangian particle scheme gives a good agreement with theoretical value of variances for conserved variables, which guarantee that the scheme is able to accurately represent fluctuation in equilibrium flow.

It has already been mentioned in earlier literature that the ability of continuum model to accurately capture the fluctuation is very much sensitive to the construction of numerical scheme. Therefore, to construct a meshfree frame work for LLNS model becomes much more complicated because of a quite arbitrary distribution of particle. Minor changes in implementation leads to significant changes in accuracy and behaviour. Future work can be extended to some other non-equilibrium scenario and higher dimension for which the stochastic stress fluxes are more complex.

REFERENCES


THE NORMALIZED QUADRATURE METHOD OF MOMENTS COUPLED WITH FINITE POINTSET METHOD

Timo F. Wächtler¹, Jörg Kuhnert², Menwer Attarakih³, Sudarshan Tiwari¹, Axel Klar¹ and Hans-Jörg Bart⁴

¹Fachbereich Mathematik
Technische Universität Kaiserslautern
POB 3049, 67653 Kaiserslautern, Germany
e-mail: waechtler@mathematik.uni-kl.de, klar@mathematik.uni-kl.de, tiwari@mathematik.uni-kl.de, www.mathematik.uni-kl.de

²Fraunhofer Institut für Techno- und Wirtschaftsmathematik (ITWM)
Fraunhofer Institut für Techno- und Wirtschaftsmathematik
Fraunhofer Platz 1, 67663 Kaiserslautern, Germany
e-mail: joerg.kuhnert@itwm.fraunhofer.de, www.itwm.de

³Faculty of Eng. Tech. Chem. Dept.
Al-Balqua Applied University
POB 15008, 11134 Amman, Jordan
e-mail: attarakih@yahoo.com

⁴Lehrstuhl für thermische Verfahrenstechnik
Technische Universität Kaiserslautern
Gottlieb-Daimler-Strasse, 67663 Kaiserslautern, Germany
e-mail: bart@mv.uni-kl.de

Key words: Population Balance Equation, FPM, NQMOM, OPMSP

Abstract. This work reports the numerical performance of the Normalized Quadrature Method of Moments (NQMOM) involving more than one quadrature node (secondary particle) for dispersed phase flows coupled with the Finite Pointset Method (FPM). At first, the model used for the dispersed phase acting in a continuous environment is discussed briefly, followed by a theoretical discussion of NQMOM and FPM. Further sections report the numerical performance for test problems with increasing difficulty.

1 INTRODUCTION

In many situations physical systems are governed by processes in which particles come into existence and die during time. A Population Balance Equation (PBE) is an appropriate mathematical way to formulate the behavior of these particulate processes. The PBE
describes the evolution of the distribution function over one or more extensive physical variables in space and time. In many branches of engineering such modeling approaches led to a deeper understanding of the corresponding processes such as aerosol dynamics and others cf. [6], [7], [5]. Mathematically one usually faces an Integro-PDE or ODE where only in few cases analytical solutions have been found, cf. [4], and hence numerical methods have to be used. Among other schemes the concept of primary and secondary particles has proven to be very promising since many schemes are discovered to be special cases of this method. This concept uses low order moments of the distribution function for reconstruction, cf. [1]. In practice, many implementations suffer from a low overall number of particles. This work reports the numerical performance of a modified version of the concept of primary and secondary particles. Its name is the ”Normalized Quadrature Method of Moments” (NQMOM), which has been introduced by [2] and is now extended to two secondary particles and one primary particle while coupled with the Finite Pointset Method (FPM) software package from the Fraunhofer Institute for Industrial Mathematics (ITWM). In the case presented here, the equation models droplets merging and breaking in a continuous fluid. One faces such multiphase flow situations for instance in liquid-liquid-contactors cf. [3].

2 THE MODEL FOR THE DISPERSED PHASE

At first, we will present the model used for the droplets and will give a look on the coupling with the solver for the continuous phase. In the following, we will call the phase consisting of the droplets the dispersed phase. As mentioned before the physical behavior of the dispersed phase, i.e. the change of the physical variables being involved can be described by the PBE. Such physical variables may be the volume of the droplets, their diameter or some solute concentration of the droplets. Here, we involve one physical variable, the volume $v$. Then, the distribution function $f = f(t, x, v)$ carries the physical information of the droplets in a way such that $f(t, x, v)dv$ is the number of all droplets at position $x$ having the volume $v$ at time $t$. $f$ satisfies the following transport equation, called Population Balance Equation

\[ \partial_t f + \nabla_x \cdot (v_d f) = \frac{1}{2} \int_0^{v_{\text{max}}} \omega(v - v', v') f(t, x, v - v') f(t, x, v') dv' - f(t, x, v) \int_v^{v_{\text{max}}} \omega(v, v') f(t, x, v') dv' - \Gamma(v) \cdot f(t, x, v) + \int_v^{v_{\text{max}}} \Gamma(v') \cdot \beta(v | v') f(t, x, v') dv' . \]

(1)

$v_d$ denotes the velocity field of the droplets, and $\Gamma$, $\beta$ as well as $\omega$ model the breakage and merging behavior of the droplets.

The functions $\Gamma$ and $\beta$ in eq. (1) are called breakage functions since they govern the breakage behavior of the droplets. $\beta(v | v')$ is the daughter droplet distribution function.
That means $\beta(v|v') dv' dv$ represents the number of droplets of volume $v$ formed by a droplet of volume $v'$ at a breakage event. There are several models for $\beta$ in literature, but all of them have in common that $\beta(v|v') = 0 \ \forall \ v' < v$ since a droplet with volume $v'$ cannot produce a droplet of volume $v$ satisfying $v' < v$ at breakage. $\beta(v|v')$ is a product of $\psi(v|v')$ and $\phi(v')$. $\psi(v|v')$ represents the density of the probability that a mother droplet of volume $v'$ actually produces a daughter droplet of size $v$ at breakage. On the other hand $\phi(v')$ is the average number of daughter droplets which are being born when a mother droplet of size $v'$ is splitting up. $\Gamma$ is said to be the breakage frequency standing for the number of breakage events per unit time. $\omega(v, v')$ is the aggregation frequency representing the number of aggregation events of a pair of droplets of size $v$ and $v'$ per unit time.

As for the breakage functions $\Gamma$ and $\beta$, there exist several formulas for the aggregation frequency. All of these formulas have to be symmetric with respect to $v$ and $v'$ in order to capture the aggregation invariance of a pair of droplets having the sizes $(v, v')$ and $(v', v)$. For both types of droplet events, breakage and aggregation, the ±-terms represent the gain and loss numbers of droplets.

The motion of the droplets within the fluid is governed by the balance of the momentum

$$\frac{d}{dt} v_d = -\nabla p + g - \frac{1}{\rho_d \alpha_d} F_{\text{drag}}$$

where $p$ denotes the pressure of the continuous liquid and $\frac{d}{dt}$ is meant to be the substantial derivative, i.e. $\frac{d}{dt} := \partial_t + v_d \partial_x$. $\alpha_d$ is the volumetric fraction and follows the conservation law $\frac{d}{dt} \alpha_d = -\alpha_d \nabla \cdot v_d$. In contrast, $\rho_d$ is the density of the dispersed phase. The model for the velocity of the dispersed phase respects the buoyancy force, influence of gravity and the drag force acting on the surface of the droplets according to a non-vanishing relative velocity $v_d - v_l$, $v_l$ being the velocity of the continuous liquid. For the drag force, the well-known model from Schiller & Naumann [8]

$$F_{\text{drag}} = \frac{3}{4} \alpha_d \rho_l C_D \frac{d_{30}}{|v_d - v_l|}\overline{|v_d - v_l|}$$

has been taken. Here $\rho_l$ is the density for the continuous fluid, in analogy to $\rho_d$, and $C_D$ is given by

$$C_D = \begin{cases} \frac{24}{Re} (1 + 0.15 \text{Re}^{0.687}) & \text{if } \text{Re} \leq 1000 \\ 0.44, & \text{otherwise} \end{cases}$$

$\text{Re}$ is supposed to be the relative Reynolds number $\text{Re} = \frac{\rho_l |v_d - v_l| d_{30}}{\mu_l}$, where $\mu_l$ is the dynamic viscosity of the continuous fluid. Note, that the intermediate diameter of the droplets, $d_{30}$, can be expressed with the help of $f$. This is the major reason for the introduction of (1). This issue will be revisited later, cf. (16).

The equation for $v_d$ is also the point of intersection for the model of the continuous phase since $F_{\text{drag}}$ involves quantities from the liquid phase and the pressure gradient $\nabla p$ itself comes from the continuous phase. Details follow in section 7.
3 THE DISCRETIZATION OF THE PHYSICAL VARIABLE

In this section we discuss the discretization of (1) with respect to $v$. In the following, the right-hand-side of (1) will be abbreviated by $s(t, x, v)$.

We perform the approach

$$f(t, x, v) = \sum_{i=1}^{N_{pp}} N_i(t, x) \delta(v - v_i(t, x))$$

where $\delta$ denotes the dirac delta distribution. The tuples $(N^i, v^i)$ are called primary particles with weight $N^i$ and volume $v^i$ and have to be computed. This is done in the following way: The range of $v$ is divided into $N_{pp}$ intervals $I_i = [v_{i-1/2}, v_{i+1/2}]$, each of them associated with one primary particle. So, $N_{pp}$ is the number of primary particles.

On this interval, we place $N_{sp}$ secondary particles $(N^i_j, v^i_j)$ that means we do the ansatz

$$f|_{I_i} = \sum_{j=1}^{N_{sp}} N^i_j(t, x) \delta(v - v^i_j(t, x)).$$

Now the average weights and volumes of the secondary particles is the primary particle, i.e.

$$N_i = \frac{\sum_{j=1}^{N_{sp}} N^i_j}{(v_{i+1/2} - v_{i-1/2})}, \quad v_i = \frac{\sum_{j=1}^{N_{sp}} N^i_j v^i_j}{\sum_{j=1}^{N_{sp}} N^i_j}$$

and the secondary particles remain to be computed.

In order to compute the secondary particles we need $2N_{sp}$ equations for each primary particle to obtain a solution for the $2N_{sp}$ unknowns $(v^i_j, N^i_j), j = 1, \cdots, N_{sp}$. Therefore we plug in the ansatz for $f|_{I_i}$ in (1), multiply by $v^r, r = 0, \cdots, 2N_{sp} - 1$ and integrate with respect to $v$.

In this way, we obtain a set of $2N_{sp}$ equations of moments

$$\partial_t \eta^r_i + \nabla_x \cdot (v^r \eta^r_i) = S^r_i, \quad r = 0, \cdots, 2N_{sp} - 1$$

using the definitions

$$\eta^r_i := \int_{v_{i-1/2}}^{v_{i+1/2}} v^r f dv, \quad S^r_i := \int_{v_{i-1/2}}^{v_{i+1/2}} v^r s(t, x, v) dv.$$

These equations have to be evaluated in space and time and after each time step the secondary particles are to be reconstructed.

For the reconstruction of the secondary particles, we use (4) and obtain the identities

$$\eta^r_i = \sum_{j=1}^{N_{sp}} v^r_j N^i_j, \quad r = 0, \cdots, N_{sp}.$$
4 THE DISCRETIZATION OF SPACE

The set of equations (5) resulting from the concept of primary and secondary particles are standard advection-reaction-equations and several schemes for hyperbolic equations can be used to resolve these equations.

Here, we use the Finite Pointset Method (FPM) to discretize the problem with respect to $x$, as it is implemented in the homonymous software package of the ITWM.

The key idea of FPM is to approximate differential operators like $\Delta$, $\nabla \cdot$, or $\partial_x$ on a set of finitely many points without grid structure.

Let

$$\Omega^p := \{ x_i : i = 1, \ldots, N \}$$

be the cloud of points where the computations are intended to be transacted. Furthermore, let

$$\Omega^p \supset \Omega^p_\xi := \{ x \in \Omega^p : r(\xi, x) < 1 \} = \{ x_l \in \Omega^p, l = 1, \ldots, m < N \}$$

be the set of neighbor particles of $\xi \in \Omega^p$ where $r(x, y)$ is a general distance function for two points $x$ and $y$.

In FPM a function $u(t, x)$ is assumed to live on $\Omega^p$ which means it uses the ansatz

$$u(t, x) = (u_1 \cdots u_N), \ u_i = u(t, x_i), \ x_i \in \Omega^p.$$  \hspace{1cm} (9)

Using the following notation for a differential operator $T$ on $\Omega^p$

$$T[u](t, \xi) := < c_\xi, u(t, x) > = \sum_{i=1}^{m} c_\xi^i u(t, x_i)$$

the two major criterions for the stencils $c_\xi$ read

- least squares criterion: $\min \frac{1}{2} \| W_\xi^{-1} \cdot c_\xi \|_2^2$
- consistency criterion: $K_\xi^T \cdot c_\xi = b$

where

$$\mathbb{R}^{m \times m} \ni W_\xi = \text{diag}(w_1^\xi, \cdots, w_m^\xi), \ w_i^\xi = w(r(\xi, x_i))$$

$$\mathbb{R}^{m \times S} \ni K_\xi = (k_\xi^0, \cdots, |k_\xi^S|).$$

$k_j^\xi, j = 0, \cdots, S$ are polynomial test functions on $\Omega^p_\xi$. They read $k_j^\xi = ((x_1 - \xi)^j, \cdots, (x_m - \xi)^j)$ and $w(r)$ is a weight function for the distance $r$.

The vector $b$ in the consistency criterion controls, which operator is approximated by $T$ and is obtained from a taylor expansion.
The FPM implementation from ITWM is designed as a Lagrangean method which tracks the solution of (5) along curves $x(t) \in \mathbb{R}^3$ with $\dot{x} = v_d$ (streamlines). Using simple computational steps (5) can be brought in a form, which is much more appropriate for Lagrangean methods since there are no more spatial differential operators to discretize:

Let $\hat{\eta}^r_i := \frac{\eta^r_i}{\eta^0_i}$ and $\hat{S}^r_i := \frac{S^r_i}{\eta^0_i}$. Then, (5) comes into

$$\frac{d}{dt} \hat{\eta}^r_i + \hat{S}^0_i \hat{\eta}^r_i = \hat{S}^r_i, \quad r = 0, \ldots, 2N_{sp} - 1$$

which are the equations we actually solve for $\hat{\eta}^r_i$. $\hat{\eta}^r_i$ are called normalized moments and these are the objects NQMOM is named after.

5 ONE PRIMARY PARTICLE AND TWO SECONDARY PARTICLE METHOD

If we run the above described method with only one primary particle, and two secondary particles we end up with the following system of equations for the dispersed phase.

$$\frac{d}{dt} v_d = - \nabla p + g - \frac{1}{\rho_d \alpha_d} F_{\text{drag}}$$

$$\frac{d}{dt} \alpha_d = - \alpha_d \nabla \cdot v_d$$

$$\frac{d}{dt} \hat{\eta}^1_1 + \hat{S}^0_0 \hat{\eta}^1_1 = \hat{S}^1_1$$

$$\frac{d}{dt} \hat{\eta}^2_2 + \hat{S}^0_0 \hat{\eta}^2_2 = \hat{S}^2_2$$

$$\frac{d}{dt} \eta^0 + \eta^0 \nabla \cdot v_d = S_0$$

$$d_{30} = \sqrt[3]{\frac{6}{\pi} \hat{\eta}^1_1}.$$  

Equation (16) is the average diameter of the droplets and is needed to evaluate the drag force in the source term for (11).

In general, equations (11)-(16) have to be solved for more than one primary particle, in order to reconstruct $f$. If the method uses only one primary particle, it is impossible to reconstruct $f$, but it provides solutions for the moments. However, the physical information is stored in the moments of $f$ and therefore the One-Primary-Two-Secondary-Particle-Method (OP2SP) is described.

Note that the system of equations (13)-(16) is free of a division by $\eta^0$ up to the evaluation of the $\hat{S}_i$’s. However, the auxiliary assumption $N_1 = N_2 := N$ that the weights of the two secondary particles $(N_1, v_1), (N_2, v_2)$ are equal changes this into a completely division-free method. This means that the method is stable even for very small numbers of droplets $\eta^0$.

The number of normalised moments $\hat{\eta}_r$ and $\eta_0$ is exactly the number of unknowns $N$, $v_1$, $v_2$. 

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6 NUMERICAL RESULTS FOR THE HOMOGENEOUS PROBLEM

Now, we report the numerical results for cases where analytical solutions have been found. These problems are homogeneous in space and breakage events are neglected.

\[
\partial_t f(t, v) = +\frac{1}{2} \int_0^{v_{\text{max}}} \omega(v - v', v') f(t, v - v') f(t, x, v') dv' \\
- f(t, v) \int_v^{v_{\text{max}}} \omega(v, v') f(t, v') dv'.
\]

For the case of a constant aggregation frequency \(\omega \equiv \text{const}\) and the sum aggregation kernel \(\omega(v, v') = v + v'\) solutions are known, cf. figure 1, figure 2. Here, we compare \(\eta_0\) and \(\eta_1\) reconstructed from \(\hat{\eta}_1\) and \(\eta_0\).

The major difficulty of solving this problem lies in the evaluation of the source term. However, approach (3), (4) respectively, yields

\[
\hat{S}_r = \frac{\eta_0^2 Nsp}{2 Nsp^2} \sum_{i,j=1}^{Nsp} [(v_i + v_j)^r - v_i^r - v_j^r] \omega(v_i, v_j), \ r = 0, 1, 2
\]

Then, the following schemes can be formulated

\[
\eta_0^{n+1} = \eta_0^n \left(1 + \Delta t \hat{S}_0^n\right),
\]

\[
\hat{\eta}_r^{n+1} = \frac{\hat{\eta}_r^n + \Delta t \hat{S}_r^n}{1 + \Delta t \hat{S}_0^n}.
\]

![Figure 1: Comparison: Numerical & analytical solutions of \(\eta_0, \eta_1\) with \(\omega = 1\) no breakage](image)

In both cases \(\eta_1\) has to be a constant because of conservation of mass whereas \(\eta_0\) has to be monotonically decreasing since the droplets are only allowed to merge and not to break.
Figure 2: Comparison: Numerical & and analytical solutions of $\eta_0$, $\eta_1$ with $\omega(v, v') = v + v'$, no breakage

7 NUMERICAL RESULTS WITH SPATIAL DEPENDENCE

Next, we encounter a 2D inflow problem with constant aggregation kernel, where the full system (11)-(16) is being solved. In parallel to that, we solve equations for the continuous phase in order to gain the quantities to evaluate the right hand side. For this phase, we consider the following momentum balance

$$\frac{d}{dt}v_l = \frac{1}{\rho_l} (\nabla \cdot S) - \frac{1}{\rho} \nabla p + g + F_{drag}^l$$

(21)

$v_l$ being the velocity, $p$ the pressure, $g$ the constant of gravity and $S$ the stress tensor which reads

$$\mu_l \frac{1}{2} \left[ \nabla v_l + (\nabla v_l)^T - \frac{1}{3} (\nabla \cdot v_l) \text{Id} \right]$$

(22)

Supposed $v_l$ to be known one can establish equations for the pressure $p = p_{hyd} + p_{dyn}$

$$\nabla \cdot \left( \frac{1}{\rho_l} \nabla p_{hyd} \right) = \nabla \cdot \left( g + F_{drag}^l \right)$$

$$\nabla \cdot \left( \frac{1}{\rho_l} \nabla p_{dyn} \right) = -\frac{d}{dt} (\nabla \cdot v) - h(v) + \nabla \cdot \left( \frac{1}{\rho_l} \nabla \cdot S \right)$$

where $h(v) = \nabla \cdot \left( \frac{d}{dt} v_l \right) - \frac{d}{dt} \nabla \cdot v_l$. These equations are used to provide the information which are needed to evaluate the dispersed phase equations. Solving equation for $p_{dyn}$ is not
straight forward since for the time step $n + 1$ we would need $v^n_{l+1}$. This problem is solved by a correction technique, where we rework the pressure approximation $\hat{p} = p_{hyd}^n + p_{dyn}^n$.

$F_{drag}$ reads

$$F_{drag}^l = C_D \frac{3}{4} |v_d - v_l| (v_d - v_l) \frac{\alpha_d}{d_{30}}$$

which comes from the overall drag force acting between the continuous and the dispersed phase at position $x$ at time $t$. In contrast, $F_{drag}$ in (2) is the drag force of a single droplet.

Solving the two phase flow problem now is done in the following way: First, we establish two separated clouds of spatial points. Each of these clouds are associated to one flow phase and moved by the evaluated corresponding velocity field.

These two clouds of points exchange information by interpolating the quantities from one cloud on the other cloud. In this way, we are capable to gather the quantities which are necessary to evaluate the right hand side of (11).

The additional terms in (15) resulting from a present velocity field are resolved by traditional methods for hyperbolic equations adapted to the meshfree framework (artificial viscosity). The iteration for (11) uses an exponential approach. We rearrange (11) into the general form

$$\frac{d}{dt} v_d + A v_d = B$$

and assume $A$, $B$ to be constant in one time step. Then, we use the analytic solution of (24) to perform a time step $dt$.

$$v_{d}^{n+1} = \frac{B}{A} + (\frac{v_{d}^n - B}{A}) \exp (-A dt)$$
Figure 4: \(d_{30}\) inlet: \(t=0.99\ \omega \equiv 10^{-8}\), no breakage, gravity acts in direction \(←\).

Figure 5: \(d_{30}\) inlet: \(t=1.50\ \omega \equiv 10^{-8}\), no breakage, gravity acts in direction \(←\).
Figure 6: velocity: magnitude and direction, $t=0.99 \, \omega = 10^{-8}$, no breakage, gravity acts in direction $\leftarrow$

Figure 7: velocity: magnitude and direction, $t=1.50 \, \omega = 10^{-8}$, no breakage, gravity acts in direction $\leftarrow$
Table 1: Parameters for the numerical results

| \( \rho_c \) | 1000 kg/m³ |
| \( \rho_l \) | 800 kg/m³ |
| \( \mu_l \) | 10⁻³ Ns/m² |

The numeric results for \( d_{30} \) indicate a qualitative correct behavior. As time proceeds the values are getting transported due to \( \partial_t + v_d \nabla x \) and increase slightly. This increase happens by virtue of the neglect of breakage events, which means that the droplets are only allowed to merge and not to split up. This implies that the average diameter has to increase.

REFERENCES


COUPLING OF GRANULAR MEDIA AND FLUID FLOW SOLVED BY THE FINITE POINTSET METHOD

Jan Marburger* and Jörg Kuhnert*

*Fraunhofer Institute for Industrial Mathematics
Fraunhofer-Platz 1
67663 Kaiserslautern, Germany
e-mail: {marburger,kuhnert}@itwm.fhg.de

Key words: Finite Pointset Method, Granular Materials, Fluid Flow

Abstract. In this paper we present strategies of simulating particles with mass like stones or dust in flow problems. The focus will be on the modelling of the particles, e.g. particle-particle and particle-wall collisions, and the coupling of the fluid phase to the particles. The latter means the interpolation of the fluid or gas phase data, provided by the finite pointset method, and the granular phase. Note that there is a large difference in density of the point set needed for the fluid phase and the one describing the granular phase. Therefore, an efficient interpolation algorithm is shown in order to decrease the numerical effort. Moreover, the modelling of an inner energy, modelling stress in the particles, is described which also allows a breakage of particles if the stress becomes to large.

1 Introduction

In many industrial processes the simulation of granular media is of great interest. For example crushing of rocks, which can be considered as particles in a gas flow or the mixing of concrete, which yields particles in a fluid flow, cf. figure 1. Very often the fluid flow involves also free boundaries, for example figure 1(a), or moving domains, like for mixing applications. Especially these problems can be solved by particle methods, like the finite pointset method (FPM), very efficiently. For this reason, we investigate the coupling of a particle phase with a fluid phase solved by FPM.

First, we state the model used for the particle phase, that is, particle-particle, particle-wall and particle-fluid interaction. Second we introduce the idea of the finite pointset method and the numerical implementation of the fluid phase.

Then the coupling is investigated. In particular we show the algorithm for mapping the fluid data to the particle phase and state the numerical implementation. We also introduce a model for an inner energy based on the total kinetic energy which allows the
consideration of internal stresses of the particles. If this stress becomes too large, the particle breaks.

Finally, the derived model is applied to a 2D particle separator.

2 Model for the Granular Phase

In this section we introduce models for the granular phase which are mainly based on [2]. First we consider particle-particle interactions followed by particle-wall interaction. Finally, the force of the fluid to the particles is taken into account. For reasons of simplicity we assume the particles to be spheres.

2.1 Particle-Particle Interaction

In this paper we use a hard sphere model, cf. [2, p.129], which is based on the integrated Newtonian equations. In the following, we denote the pre-collision quantities by \( \cdot \), e.g. the pre-collision velocity is denoted by \( \bar{v}_1 \) and the post-collision one by \( v_1 \). The contact phase is illustrated in figure 3. For spheres with homogeneous density we obtain the conditions

\[
\begin{align*}
m_1(v_1 - \bar{v}_1) &= J \\
m_2(v_2 - \bar{v}_2) &= J \\
I_1(\omega_1 - \bar{\omega}_1) &= r_1 n \times J \\
I_2(\omega_2 - \bar{\omega}_2) &= r_2 n \times J
\end{align*}
\]

where \( v \) denotes the velocity of the particle, \( \omega \) the angular velocity, \( J \) the impulsive force and \( n \) the normal vector pointing from particle 1 to 2. The material parameters are the radius \( r \), the mass \( m \) and the moment of inertia \( I \).

We define the relative velocity of the particles and at the contact point by

\[
G := \bar{v}_1 - \bar{v}_2 \quad \text{and} \quad G_c := G + r_1 \bar{\omega}_1 \times n + r_2 \bar{\omega}_2 \times n
\]

respectively. The tangential velocity and tangential vector is then given by

\[
G_{ct} = G_c - (G \cdot n)n \quad \text{and} \quad t = \frac{G_{ct}}{|G_{ct}|}.
\]
During the contact the particles can slide the whole contact time or stop sliding during
the collision. These two cases are distinguished by the relation
\[
\frac{\mathbf{G} \cdot \mathbf{n}}{|\mathbf{G}_{ct}|} < \frac{2}{7(1 + e)f}
\]
where \(e\) is the restitution coefficient and \(f\) the friction coefficient, which are given material
parameters. If condition (1) is satisfied, the particles slide during the contact and we
obtain the post collision quantities
\[
\mathbf{v}_1 = \tilde{\mathbf{v}}_1 - (\mathbf{n} - ft)(\mathbf{G} \cdot \mathbf{n})(1 + e)\frac{m_2}{m_1 + m_2}
\]
\[
\mathbf{v}_2 = \tilde{\mathbf{v}}_2 + (\mathbf{n} - ft)(\mathbf{G} \cdot \mathbf{n})(1 + e)\frac{m_1}{m_1 + m_2}
\]
\[
\mathbf{\omega}_1 = \tilde{\mathbf{\omega}}_1 - \frac{5}{2r_1}(\mathbf{G} \cdot \mathbf{n})(\mathbf{n} \times \mathbf{t})(1 + e)f\frac{m_2}{m_1 + m_2}
\]
\[
\mathbf{\omega}_2 = \tilde{\mathbf{\omega}}_2 - \frac{5}{2r_2}(\mathbf{G} \cdot \mathbf{n})(\mathbf{n} \times \mathbf{t})(1 + e)f\frac{m_1}{m_1 + m_2}
\]
If condition (1) is not satisfied, the particles stop sliding during the contact and we obtain
\[
\mathbf{v}_1 = \tilde{\mathbf{v}}_1 - (\mathbf{G} \cdot \mathbf{n})(1 + e)\mathbf{n} + \frac{2}{7} |\mathbf{G}_{ct}| \mathbf{t} \frac{m_2}{m_1 + m_2}
\]
\[
\mathbf{v}_2 = \tilde{\mathbf{v}}_2 + (\mathbf{G} \cdot \mathbf{n})(1 + e)\mathbf{n} + \frac{2}{7} |\mathbf{G}_{ct}| \mathbf{t} \frac{m_1}{m_1 + m_2}
\]
\[
\mathbf{\omega}_1 = \tilde{\mathbf{\omega}}_1 - \frac{5}{7r_1} |\mathbf{G}_{ct}| (\mathbf{n} \times \mathbf{t}) \frac{m_2}{m_1 + m_2}
\]
\[
\mathbf{\omega}_2 = \tilde{\mathbf{\omega}}_2 - \frac{5}{7r_2} |\mathbf{G}_{ct}| (\mathbf{n} \times \mathbf{t}) \frac{m_1}{m_1 + m_2}
\]
For further details we refer to [2].

2.2 Particle-Wall Interaction

The particle-wall interaction is more complex than the particle-particle interaction. On
the one hand we have to distinguish the sliding and non-sliding cases, similar to the above
case. On the other hand, the handling also depends on the geometry. First, we consider
the geometrical properties. In three dimensions a ball can hit either a surface, edge or
corner. If a ball hits a corner point or an edge then we set the normal vector \(\mathbf{n}\) according
to figure 2 and use the particle-particle approach shown above. In particular, particle 1
is the approaching one and particle 2 is a ghost particle at the contact point. This ghost
particle models the wall by setting \(r_2 = 0, v_2 = 0, \omega_2 = 0\) and \(m_2 = \infty\), i.e. very large.

In the case that a particle hits a surface we define the normal and tangential directions by
\[
\mathbf{N} = \mathbf{n}, \quad \mathbf{T} = \mathbf{v} - (\mathbf{v} \cdot \mathbf{n})\mathbf{n} \quad \text{and} \quad \mathbf{S} = \mathbf{N} \times \mathbf{T}
\]
and denote by \( v_T := \mathbf{v} \cdot T/|T| \) the quantity in the corresponding direction. Similar to the particle-particle interaction, we have to distinguish the sliding and non-sliding case which yields the following post-collision quantities. If

\[
\frac{v_N}{|\mathbf{v}|} < -\frac{2}{7f(e+1)}
\]

is satisfied we obtain

\[
\begin{align*}
v_T &= \frac{5}{7} \left( \bar{v}_T - \frac{2r}{5} \bar{\omega}_S \right) \\
v_N &= -e\bar{v}_N \\
v_S &= \frac{5}{7} \left( \bar{v}_S + \frac{2r}{5} \bar{\omega}_T \right)
\end{align*}
\]

otherwise

\[
\begin{align*}
v_T &= \bar{v}_T + f(e+1)\bar{v}_N \\
v_N &= -e\bar{v}_N \\
v_S &= \bar{v}_S \\
\omega_T &= \bar{\omega}_T \\
\omega_N &= \bar{\omega}_N \\
\omega_S &= \bar{\omega}_S + \frac{5}{2r}f(e+1)\bar{v}_N.
\end{align*}
\]

Again we refer to [2] for more details.

### 2.3 Particle-Fluid Interaction

In this paper we only consider the influence of the fluid and the surrounding to the particles, not vice versa. First, we consider the gravity \( \mathbf{g} \). The force on the particle is given by \( \mathbf{F}_{\text{part}} = m\mathbf{g} \). This yields, by neglecting collisions, the relation \( \mathbf{v}_{\text{part}} = \mathbf{g} \). Similarly, the force induced by the fluid is handled. Here we obtain \( \mathbf{F}_{\text{part}} = \alpha(\mathbf{v}_{\text{fluid}} - \mathbf{v}_{\text{part}}) \), where \( \alpha \) is a material constant depending on the properties of the fluid and the particle. In a similar manner other forces, e.g. the Magnus force, can be modelled.
3.1 Finite Pointset Method

The basic idea of this method is exemplified by the Laplacian. Let \( \Omega \subset \mathbb{R}^2 \) be a bounded domain and \( f : \Omega \to \mathbb{R} \) a sufficiently smooth function. Moreover, let \( P = \{x_1, \ldots, x_N\} \), \( x_i = (x_i, y_i) \in \Omega \) denote a given point set. Then we approximate \( f \) by \( f_h(x) = \sum_{j=1}^{N} c_j(x) f_j \) where \( c_j \) are approximation weights and \( f_j = f(x_j) \) supporting values. For the Laplacian we get

\[
\Delta f(x) \simeq \Delta \left( \sum_{j=1}^{N} c_j(x) f_j \right) = \sum_{j=1}^{N} (\Delta c_j(x)) f_j = \sum_{j=1}^{N} \tilde{c}_j(x) f_j.
\]

To obtain the weights \( \tilde{c}_j \) we use the following properties of the continuous Laplacian

\[
\Delta \text{const} = \Delta x = \Delta y = \Delta(xy) = 0 \quad \text{and} \quad \Delta(x^2) = \Delta(y^2) = 2.
\]

Hence, for each point \( x_j \in P \) the weights \( \tilde{c}_j(x) \) have to satisfy

\[
\sum_{j=1}^{N} \omega_j(x) \tilde{c}_j(x) = 0, \quad \sum_{j=1}^{N} \omega_j(x) \tilde{c}_j(x)(x-x_j)(y-y_j) = 0, \quad \sum_{j=1}^{N} \omega_j(x) \tilde{c}_j(x)(x-x_j) = 0
\]

\[
\sum_{j=1}^{N} \omega_j(x) \tilde{c}_j(x)(y-y_j) = 0, \quad \sum_{j=1}^{N} \omega_j(x) \tilde{c}_j(x)(x-x_j)^2 = 2, \quad \sum_{j=1}^{N} \omega_j(x) \tilde{c}_j(x)(y-y_j)^2 = 2
\]

in a neighbourhood of \( x \), which is defined by the smoothing length (cf. figure 4), and the weighting functions \( \omega_j(x) \) depending on the distance from \( x \) to \( x_j \), e.g. a Gaussian function as shown in figure 5. This finally yields an underdetermined linear system, as we use more supporting points than approximation conditions. The resulting system is solved by a QR factorisation, for instance.

In this fashion, all spatial derivatives are approximated. Also complex boundary conditions can be implemented in that way. For example, the derivative in normal direction, i.e. \( \nabla f \cdot n \), can be approximated by the conditions

\[
\nabla \text{const} \cdot n = 0, \quad \nabla x \cdot n = n_x \quad \text{and} \quad \nabla y \cdot n = n_y
\]

Figure 4: Point set and smoothing length \( h \).

Figure 5: Weight function.

Figure 6: Illustration of \( h_{fluid} \) and \( h_{part} \).
for $n = (n_x, n_y)^T$. Moreover, the extension of the above approach to 3D is straightforward, i.e. appropriate conditions for the $z$-direction are added. For more details we refer to [3, 4].

3.2 Numerical Implementation of the Navier-Stokes Equation

The fluid phase is modelled by the incompressible Navier-Stokes equation which is roughly given by

$$\frac{\partial}{\partial t} u + u \cdot \nabla u - \nu \Delta u = -\nabla p \quad \text{in } \Omega \times (0, T) \quad (3a)$$

$$\text{div } u = 0 \quad \text{in } \Omega \times (0, T) \quad (3b)$$

$$u = g \quad \text{on } \Gamma \times (0, T) \quad (3c)$$

where $g$ satisfies the compatibility condition $\int_{\Gamma} g \cdot n \, d\omega(x) = 0$. Moreover, feasible initial conditions are given. We decouple the velocity $u$ and pressure $p$ in the momentum equation (3a) and discretise it in time, i.e.

$$\frac{1}{\tau} (u^n - u^*) + u^* \cdot \nabla u^* - \nu \Delta u^* = 0 \quad \text{in } \Omega$$

$$u^* = g \quad \text{on } \Gamma. \quad (4)$$

Then we obtain for the pressure

$$\frac{1}{\tau} (u^{n+1} - u^*) = -\nabla p \quad \text{in } \Omega. \quad (5)$$

Taking the divergence of (5) yields

$$\text{div } u^{n+1} - \text{div } u^* = -\tau \Delta p \quad \text{in } \Omega.$$ 

To satisfy equation (3b) we set $\text{div } u^{n+1} = 0$ and obtain the pressure correction equation

$$\Delta p = \frac{1}{\tau} \text{div } u^* \quad \text{in } \Omega$$

$$\nabla p \cdot n = 0 \quad \text{on } \Gamma.$$

Finally, we derive $u^{n+1}$ by using the pressure $p$ in (5) and obtain

$$u^{n+1} = u^* - \tau \nabla p.$$

This method is known as Chorin’s projection method [1]. Note that the pressure correction equation is ill-posed. To get a well-posed system we add a regularisation, e.g. $\int_{\Omega} p \, dx = 0$. Note that it is possible to decouple the convection and diffusion equation in (4) which yields the numerical scheme shown in algorithm 3.1.
Solve convection by moving point set

\[ \vec{X}^{(n+1)} = \vec{X}^{(n)} + \tau \vec{u}^{(n)} \]

Solve velocity equation

\[ \frac{1}{\tau} (\vec{u}^{(n+\frac{1}{2})} - \vec{u}^{(n)}) = \Delta h_{X} \vec{u}^{(n+\frac{1}{2})} \]

Solve pressure equation

\[ \Delta h_{X} \vec{p}^{(n+1)} = \frac{1}{\tau} \nabla h_{X} \cdot \vec{u}^{(n+\frac{1}{2})} \]

Correct velocity

\[ \vec{u}^{(n+1)} = \vec{u}^{(n+\frac{1}{2})} - \tau \nabla h_{X} \vec{p}^{(n+1)} \]

Algorithm 3.1: One time step of Chorin’s projection with FPM. The point set is denoted by \((\vec{X}, \vec{u}, \vec{p}) = \{(X_i, u_i, p_i)\}_i\). Here \(X_i\) denotes the position of particle \(i\) and \(u_i\) and \(p_i\) the corresponding velocity and pressure.

| \(h_{\text{fluid}}\) and \(h_{\text{part}}\) denote the discrete (FPM) counterparts to \(\Delta\) and \(\nabla\) w.r.t. the point set \(\vec{X}^{(n+1)}\). The above equations are equipped with the corresponding boundary conditions. |

4 Coupling Method

In this section we show the numerical implementation of the coupling of the fluid and the particle phase. We initialise the domain with two point sets. One is used for solving the fluid phase with smoothing length \(h_{\text{fluid}}\), the other represents the initial distribution of the particles with an average distance of \(h_{\text{part}}\). Note that \(h_{\text{fluid}}\) is fixed during the simulation whereas \(h_{\text{part}}\) changes, i.e. we obtain regions without particles and regions with a very dense distribution.

4.1 Mapping of Fluid Data to the Particle Phase

In a region we have the two possibilities \(h_{\text{fluid}} < h_{\text{part}}\) and \(h_{\text{fluid}} > h_{\text{part}}\). In the first case, we have more calculation points for the fluid phase than particles in a region as illustrated in figure 6 where the red (large) points represent the particle phase and the blue (small) ones the fluid phase. Here, the most efficient way is the mapping of the fluid phase data to each particle by deriving the interpolation coefficients at the position \(x_{\text{part}}\) as described in section 3.1. The fluid points needed for the approximation lie in the inner circle (figure 6).

If we have much more particles than fluid points, illustrated by figure 6 where now red is the fluid phase and blue the particle phase, this method would not be very efficient as we derive for each particle the approximation coefficients. Here, it is much more efficient to calculate an approximation polynomial using the fluid points marked by the outer circle which is used to approximate the particle quantities. In particular, this polynomial is, roughly speaking, derived by \(f(x) := ax^2 + bx + c\) with the conditions \(f(x_i) = f_i\) for all
fluid points $i$. Since we have more equations than unknowns, we obtain an overdetermined system. The resulting function $f$ is used to map the desired quantity to the particle phase by $f_{part} := f(x_{part})$.

### 4.2 Numerical Implementation of the Coupling

The numerical implementation of the time step $n + 1$ is organised as follows.

1. The fluid phase is solved for the velocity field $v_{fluid}^{(n+1)}$ and the pressure $p_{fluid}^{(n+1)}$.
2. The values of the fluid phase are mapped to the particle phase, cf. section 4.1.
3. The acting forces are added by setting $v_{part}^{(n+1)} = v_{part}^{(n)} + \tau F(v_{fluid}^{(n+1)}, p_{fluid}^{(n+1)}, \ldots)$, where $\tau$ denotes the time step and $F$ a function describing the particle force.
4. All particle-wall contacts are resolved according in section 2.2. In particular, each particle is checked for a wall contact in the current time step by neglecting all other particles, that is, no particle-particle contact is taken into account. If a contact occurs it is resolved and this particle will no longer be considered.
5. The remaining particles are checked for particle-particle interactions. If a contact occurs, the two particles are moved to the contact position, then the contact is resolved and finally, a particle-wall contact detection is performed. All particles with contact are moved to their final position for the current time step and will no longer be checked for interactions.
6. All remaining particles, which did not have a contact, are moved to their final position according to $v_{part}^{(n+1)}$.

Especially for large time steps it is not possible to resolve all contacts and we allow a few particles to fly through each other. Since we only want to consider small particles later on, which also guarantees an appropriate particle distance, this is an acceptable behaviour. If too many particle contacts cannot be resolved, the time step has to be reduced. Note that resolving all contacts for a huge amount of particles in the system would be very expensive but not necessary to obtain a qualitatively good result for the particle phase.

### 4.3 Handling of the Total Kinetic Energy

The model of the particle-particle and -wall interaction also includes the coefficient of restitution. Hence, the total kinetic energy $E_{kin} = \frac{1}{2} \sum_{i=1}^{2} m_i |v_i|^2 + I_i |\omega_i|^2$ before the collision can be larger than the post-collision one. This difference is used to define an inner energy $e_i$ for each particle. If this inner energy is too large, i.e. greater than a given threshold, the particle breaks into two parts. The breakage is modelled as a post-processing step. We reduce the radius and mass of the particle $i$ by $r_i^{(n+1)} = \sqrt[3]{\frac{1}{2}} r_i^{(n)}$ and $m_i^{(n+1)} = \frac{1}{2} m_i^{(n)}$. Then a new particle $j$ is generated by copying particle $i$. Finally, we rotate the velocity and angular velocity vector by random angles $\alpha, \beta$ and $\gamma$ about the
Figure 7: Breakage of a particle. In the beginning, only the blue particle moves. After the collision, the inner energy of the green ball gets large enough for a breakage. The lines represent the traces.

\[ x, y, \text{ and } z \text{-axis, respectively. Note that the angles should be greater than } 0^\circ \text{ and much less than } 90^\circ. \text{ Hence, we obtain} \]

\[ v_i^{(n+1)} = R(\alpha, \beta, \gamma)v_i^{(n)} \]
\[ \omega_i^{(n+1)} = R(\alpha, \beta, \gamma)\omega_i^{(n)} \]
\[ v_j^{(n+1)} = R(-\alpha, -\beta, -\gamma)v_i^{(n)} \]
\[ \omega_j^{(n+1)} = R(-\alpha, -\beta, -\gamma)\omega_i^{(n)} \]

where \( R \) denotes the rotation matrix. Note that this is just a rough approximation but conserves the total kinetic energy. An example of applying this scheme is shown in figure 7.

Due to numerical issues also an increase of the total kinetic energy can occur which would increase rapidly over time. To avoid this case, \( E_{kin} \) is checked after each collision. If it increases, we scale the post-collision velocities and angular velocities until \( E_{kin} < \bar{E}_{kin} \) where \( \bar{E}_{kin} \) denotes the pre-collision energy.

5 Numerical Results

The model we have introduced is tested for a simple 2D particle separator, which separates light particles from heavy ones by a fluid flow. The schematic domain is shown in figure 8. The fluid inflow is on the left with an outlet on the right. The remaining boundaries are walls. Every 0.1s particles are injected at the top of the geometry which can leave the separator to the right and the bottom wall. For testing, the injected particles have variable mass which increases from the left to the right. Moreover, gravity is acting on the particles.

The results are shown in figure 9. The fluid flow is represented by streamlines. The heavy particles located at the right are mostly driven by gravity and not affected by the fluid flow strongly. In contrast, the light particles follow the fluid flow quickly until a collision occurs. The simulation shows that most light particles leave the separator to the right but there is also a certain amount of particles leaving the domain at the bottom due to collision with heavier particles.

6 Conclusion

For most applications the presented algorithm is sufficient and yields qualitatively good results. Since it does not resolve all particle-particle contacts, a huge amount of expensive
tests can be neglected which yields a very efficient algorithm for solving fluid-particle interactions. Also the presented mapping method increases the speed of the algorithm if we consider much more particles than calculation points for the fluid. This occurs for example in the simulation of dust in a gas flow. Moreover, the possibility of considering breakage is very useful for crushing processes.

REFERENCES
Figure 9: Simulation of a particle separator. Particles, whose weight increases from the left to the right, enter the device from above every 0.1s. The background lines show the streamlines of the fluid flow. The time series goes from the left to the right for $t = 0, \ldots, 4$. 
MODELLING OF INTERNAL STRESSES IN GRINDING CHARGES

PÄR JONSÉN*, BERTIL I. PÅLSSON† AND HANS-ÅKE HÄGGBLAD *

* Division of Mechanics of Solid Materials
  Luleå University of Technology
  SE-97187 Luleå, Sweden
  e-mail: Par.Jonsen@ltu.se, www.ltu.se/staff/p/parj
  e-mail: Hans-Ake.Haggblad@ltu.se, www.ltu.se/staff/h/hah

† Division of Sustainable Process Engineering
  Luleå University of Technology
  SE-97187 Luleå, Sweden
  e-mail: Bertil.Palsson@ltu.se www.ltu.se/staff/p/palle

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Summary. Physically realistic methods are a necessity to close the gap between reality and numerical result in modelling of tumbling mills. A problem is that tumbling mills often operate in a metastable state because of the difficulty to balance the rate of replenishment of large ore particles from the feed with the consumption in the charge. Understanding of the charge motion within the mill is of significance in mill optimisation. Both the breakage of ore particles and the wear of liners/ball media are closely linked to the charge motion. In this work, a ball charge and its interaction with the mill structure is modelled with the smoothed particle hydrodynamic (SPH) method. The mesh free formulation and the adaptive nature of the SPH method result in a method that handles extremely large deformations and thereby suits modelling of grinding charges and pulp liquids. The flexible rubber lifter and the lining are modelled with the finite element method (FEM). A hyper-elastic model governs the elastic behaviour of the rubber.

The comminution process is complex and to include all phenomena that occur in a single numerical model is today not possible. Therefore, modelling the physical interaction between charge, mill structure and pulp liquid is the major goal in this work. The SPH-FEM model can predict responses of the mill structure e.g. stress and strain. All parts of the mill system will affect its response and the model gives the opportunity to study the influence of the mill structure and e.g. pressure and shear stresses in the charge. This computational model also makes it possible to predict, the contact forces for varying mill dimensions, liner combinations and pulp densities. By comparing numerical results with experimental measurement from grinding in a pilot mill equipped with an instrumented rubber lifter a validation is done. The deflection profile of the lifters obtained from SPH-FEM simulation shows a reasonably good correspondence to pilot mill measurements as measured by an embedded strain gauge sensor. This model gives information on the grinding process in tumbling mills and better correlation with experimental measurements.
1 INTRODUCTION

Grinding of material in tumbling mills is a highly important size reduction process for the mining industry. The process is difficult to control and energy inefficient. The grinding process in a tumbling mill is strongly connected to the charge properties, liner design, rotational speed, filling rate, pulp fluid properties etc. Both the breakage of ore particles and the wear of liners/ball media are closely linked to the charge motion. To study these phenomena in a physically correct manner, suitable numerical models for different parts of the mill system has to be utilised. Validation of these models is of major importance.

A traditional approach to study the charge behaviour is to use the discrete element methods (DEM). The method was introduced by Cundall [1] for analyses of rock mechanic problems. When applied to comminution it gives an opportunity to study several aspects of grinding in detail than has been possible to date, e.g. charge viscosity and charge size distribution, collision forces, energy loss spectra and power consumption. An initial attempt to use DEM to describe the interaction of large grinding balls and the lining was presented by Rajamani [2]. However, some improvements of today’s DEM models can be identified; for example, charge normal and shear stress can not be found with rigid DEM particles. Jonsén et al. [3] took one step towards a more physically realistic mill model. They used a combined DEM-FEM model to study the interaction between the charge and the mill structure.

For astrophysical problems in open space, the smoothed particle hydrodynamics (SPH) method was invented, see [4,5]. It is a mesh free, point based method for modelling fluid flows, which has been extended to solve problems with material strength. Today, the SPH method is used in many areas such as fluid mechanics (for example; free surface flow, incompressible flow and compressible flow), solid mechanics (for example; high velocity impact and penetration problems) and high explosive detonation over and under water. In the SPH method, a problem domain is represented by a set of particles or points, see [6]. Besides representing the problem domain, the points also act as the computational frame for the field approximation. Each point is given a mass and carries information about spatial coordinate, velocity, density and internal energy. Other quantities as stresses and strains are derived from constitutive relations. The mesh free Lagrangian formulation and the adaptive nature of the SPH method result in a method that handles extremely large deformations. In this work, a step towards a physically correct description of the ball charge is taken by using SPH to model the ball charge.

One of the most developed numerical methods is the finite element method (FEM). FEM is a numerical solution method based on continuum mechanics modelling, a constitutive relation for the actual material is described and the governing equations are solved [7]. Varieties of different constitutive models for a large number of materials are implemented in modern finite element (FE) code. A material model approximates a real physical behaviour. The comminution process is complex and to include all phenomena that occur in a single numerical model is today not possible. Therefore, modelling the physical interaction between the charge and the mill structure is important if the internal stress in the charge is studied. The SPH-FEM model can predict the classical DEM results, but can also predict responses from
the mill structure like, e.g., stress and strain, see [8]. All parts of the mill system will affect its response and a SPH-FEM model gives the opportunity to study the pressure and shear stresses in the charge. In this work the internal stresses in the charge is studied, as it may give a better understanding of the grinding process. The validation of this task is done by comparing numerical results with experimental measurements from grinding in a pilot mill equipped with an instrumented rubber lifter.

2 EXPERIMENTAL MEASUREMENTS

Pilot mill experimental measurements have been done to study the interaction between the charge and lining. As the mill is rotated the charge will load and deform the lining. In the measurements, the deflection of a rubber lifter captured as it moves through the charge.

2.1 Measurement system

One lifter is equipped with a sensor and a simplified view of the sensor is shown in Fig. 1. The mill has several lifters and the one equipped with a leaf spring (marked 1) is whose deflection is measured by the strain gauge (marked 2). As the mill rotates and the lifter with the sensor dips into the charge, the force acting on the lifter increases, which in turn, causes a deflection. The strain gauge mounted on the leaf spring converts this deflection to an electric signal. This signal is amplified, filtered and transmitted to a computer. Metso Minerals have marketed the sensor system under the name Continuous Charge Measurement system (CCM), see [9]. A typical deflection profile of the sensor signal and an attempt to divide it into different segments is shown in Fig. 2. The boundaries and size of the partitions are determined by engineering knowledge of the grinding process. Each segment in Fig. 2 illustrates an important dynamic event during the passage of the sensor-equipped lifter bar under the mill charge. The ordinate in Fig. 2 shows the deflection of the lifter bar, which indirectly corresponds to the force acting on it and the abscissa is the mill rotation angle with a resolution of 1°.

Figure 1. To the right a cross section of a mill with a horizontal reference line, the left part shows the lifter bar (1) with a strain gauge sensor embedded (2), from Tano (2005).
The sensor signature reflects different charge features such as mill volume, position and behaviour of the mill charge. Both toe region (S2) and shoulder region (S6) are well known, and can be used to calculate the volumetric mill load and the angle of repose based on the CSM-signal that is calibrated against the measured charge volume when the charge is at rest. Collectively, these data give a good measure of the location of the charge. The other segments are less known but are expected to provide information about grinding efficiency. Such features can be extracted from the sensor signal for the purpose of process monitoring and diagnosis of process performance. Table 1 provides a summary of the stages during one mill revolution. The lifter bar angles given in Table 1 correspond to the positions marked in Fig. 2, as a reference in these measurements is the horizontal line, which corresponds to 0 degrees at the 9 o’clock position. In this work, an attempt is made to identify the corresponding segments in a predicted deflection profile obtained from SPH-FEM simulation. The toe/shoulder position in particular will be inspected for validation purposes.

![Figure 2. Segmentation of a typical sensor signal during its passage in the charge Tano [10].](image)

<table>
<thead>
<tr>
<th>Segment</th>
<th>Lifter bar angle</th>
<th>Process feature</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1: the sensor lifter bar (SL) is still in the air</td>
<td>&lt; 50°</td>
<td>Indicate the toe position of the charge, and if present, the slurry pool</td>
</tr>
<tr>
<td>S2: the SL hits the ball charge and starts to get submerged in the charge</td>
<td>50° - 70°</td>
<td>Rate of charge varies with mill speed</td>
</tr>
<tr>
<td>S3: the SL starts to bend forward due to turbulence in the toe area</td>
<td>70° - 85°</td>
<td>Both speed and charge level has an influence, wear of lifter</td>
</tr>
<tr>
<td>S4: the SL is at peak bending</td>
<td>75° - 90°</td>
<td>Indication of every lifter bar hitting the charge</td>
</tr>
<tr>
<td>S5: the SL is moving through the charge</td>
<td>80° - 190°</td>
<td>Indicates the shoulder position of the charge</td>
</tr>
<tr>
<td>S6: the SL has gradually decrease the bending and is at take-off position</td>
<td>190° - 215°</td>
<td></td>
</tr>
<tr>
<td>S7: the SL is leaving the ball charge and starts slowly to rise to an upright position</td>
<td>&gt; 215°</td>
<td></td>
</tr>
</tbody>
</table>
2.2 Experimental conditions

The pilot mill is 1.41 m in diameter and 1.22 m in length. It is a grate-discharge mill, equipped with 12 rubber lifters of square size 0.1 m and a face angle of 45 degrees. Steel balls with a diameter ranging between 10-30 mm and a density of 7800 kg/m$^3$ were used in the experiments. The test material, a hematite pellet feed with $d_{50}$ around 35µm and a solids density of 5200 kg/m$^3$, was chosen to get stable grinding conditions with respect to feed size variations. Feed rate was kept constant at approx. 1.5 tonne/h. Four experiments were run with the mill speed at 73% and 78% of critical speed ($n_c$) for two levels of mill filling ($J =$ 25% and 35% by volume). The embedded strain gauge sensor measured the load position (toe and shoulder) using the CCM algorithm, proprietary of Metso Minerals. More details regarding the experimental measurements can be found in [10].

3 MODELLING

To virtually reproduce a tumbling ball mill process a combined three dimensional SPH-FEM model is used. The commercial nonlinear finite element code LS-Dyna v971 R5.1 [11] has been used for the modelling and simulation of the mill. The mill structure consists of lifters, liners made of rubber, and a mantel made of solid steel. Here the rubber is modelled as a hyper-elastic material and the mill mantel is modelled as a rigid material.

3.1 SPH Charge model

The problem domain in SPH is represented by a set of particles or points. Besides representing the problem domain, the points also act as the computational frame for the field approximation. Initially, each point is given mass and coordinate information. During calculation, information about spatial coordinate, velocity, density and internal energy is stored in the each point. From constitutive relations, stresses and strains are derived. The SPH method is an adaptive Lagrangian method, which means that in every time step the field function approximations are performed based on the current local set of distributed points. Another difference from the FE method is that the points are free to move in action of the internal and external forces, there are no direct connections between them like the mesh in FE method.

The SPH method is originally a continuum-based method used to model fluids, granular and solid material. For that kind of processes the smoothing length can vary. Here, the balls are modelled in three different sizes 10, 20 and 30 mm. Each sphere size is given a mass $m$ and radius $h$ that correspond to the density of steel 7800 kg/m$^3$. To reproduce the charge behaviour the smoothing function is set to a constant value. In the present case, the ball charge is modelled with 6000 SPH particles. In 3D, a sphere represents the SPH particle with its radius controlled by the value of $h$. To model the steel balls in the charge the sphere is given a constant mass and radius. A constitutive relation eq. 1 given by the Drücker-Prager model governs the interaction between the balls.

$$ f_{dp}(p,J_2) = \sqrt{2J_2} + kp + d = 0 $$
Where, \( p \) is the mean pressure, \( J_2 \), the second invariant of the deviator stress tensor and \( k \) and \( d \) are material parameters representing internal friction and cohesion, see [11]. In this work, the slope of the internal friction \( k \) has been predicted from particle-particle friction recommended by Rajamani [2]. For simplicity, the elastic properties are set constant for the actual range of density. When the SPH particles interact with each other or the lining values of mechanical properties like stresses can be calculated. The SPH particle will give a constant value of these properties within the particle.

### 3.2 Mill structure model

A 0.10 m slice of the mill is modelled and the diameter is 1.414 m. All structural parts of the model: rubber liners, rubber lifters and mantel are modelled with eight node solid elements. This type of element is fully integrated with a reduced integration of the pressure part to avoid volumetric locking of the element. The Blatz-Ko hyper-elastic model governs the elastic behaviour of the rubber, see [12]. Hyper-elastic models are a classic approach to model rubber material as they are considered ideally elastic. Here, the stress-strain relationship derives from a strain energy density function. The supplier of the lining provided experimental data for the rubber. In Fig 3, the SPH-FEM mill model is shown.

![Figure 3. The 3D SPH-FEM mill model containing a graded charge, lifter and liners in rubber and a solid mantel modelled with rigid material](image)

### 4 RESULTS

The mill process is simulated for four revolutions that is around 10 s in real time. The charge filling was \( J = 25\% \) and speed 73\% of critical rotational speed. In Fig. 4, a snapshot of the total velocity vectors and the charge movement at steady state is shown. Note, the internal kidney-shaped rotational motion of the charge, where the grinding balls merely are holding...
their places and rotating in their positions. As the mill rotates charge motion is induced. During this motion particle-particle and particle-structure interactions occurs in the mill system. The contact between particles and structure of the mill results in a load to the structure of the mill. The structure will respond with deformation upon the incoming load from the charge. These deformations will give rise to strains and stresses which are dependent on the material properties of the structure. This load also induces mechanical waves in the whole structure and charge. Jonsén et al. [3] did show that a DEM-FEM model could predict the mechanical waves that travel in the mill structure. The SPH-FEM model can also show that mechanical waves travel in the charge. In Fig 5, the pressure distribution in the charge is shown for three different occasions within 30° including submerging, fully loaded and just before the next lifter will submerge. As the lifter submerges into the charge (position a), a pressure builds up in front of the lifter. In position b, the pressure is fully developed. Position c shows that the pressure follow the lifter as it moves in the charge. The collision that appears as the lifter submerges into the charge starts a mechanical wave that travels through the charge. As the mechanical wave travel through the system, the charge is compressed and unloaded several times. These waves creates fluctuations in the lifter load that is shown in the experimental study, see Fig 2. The highest pressure is found as the lifter goes into the charge.

![Figure 4. A snapshot of the total velocity vectors in the charge.](image-url)
Figure 5. The pressure distribution in the charge as the lifter travels through the charge. a) As a lifter submerges into the charge, hydrostatic pressure build up and a mechanical wave is induced and travels through the charge. b) A fully developed pressure region is found in front of the lifter. c) The pressure region moves with the lifter and a subsequent lifter is about to submerge into the charge.
Figure 6. The maximum shear stress distribution in the charge as the lifter travels trough the charge. a) As a lifter submerges into the charge, shear stress build up and a mechanical wave is induced and travels through the charge. b) A fully developed shear stress region is found in front of the lifter. c) The shear stress region moves with the lifter and a subsequent lifter is about to submerge into the charge.
At identical positions the maximum shear stress distribution for the mill is shown in Fig 6. As the lifter submerges into the charge (position a), a shear stress builds up in front of the lifter. In position b, the shear stress is fully developed. Position c shows that the shear stress follow the lifter as it moves in the charge. The magnitude and volume affected by the maximum shear stress seems to be smaller that for the pressure. The highest value for the shear stress is found in front of the lifter close to where the horizontal velocity changes direction. As for the pressure, the shear stress is also changing from low to high level as the mechanical waves travel in the system.

The deflection of the lifter during its fourth passage for the simulated and the experimentally measured is shown in Fig. 7. There are differences in the signature between measured and simulated results that probably are due to the lack of a dampening pulp liquid in the simulated charge model. What is important here is that both simulations show the same 30° separation between the peaks as the measured signal. This means that the mechanical waves are correctly predicted. The maximum peak values for measured and the simulated signature occurs around 105°. The charge toe angle is 69° for the measured and 65° for the model. The shoulder angle for measured is 202° and 190° for the model charge. The peaks are higher for the model.

Figure 7. Displacement of the lifter during the fourth passage, solid line represents the response from the graded charge and dashed the SPH-FEM model
5 DISCUSSION AND CONCLUSION

Through a SPH-FEM model, structural response and its influence on the charge motion in a mill can be studied in great detail. Constitutive models govern the behaviour of materials in the mill. The models are calibrated with data from experimental tests or taken from literature. The SPH-FEM model gives not only the opportunity to optimize the material selection of the mill structure but also to study the internal workings of the charge. Critical response values e.g., stress and strain can be identified during the milling process. Forces and mechanical waves in the structure and charge can be found. An attractive result is the pressure and shear stress distributions and their change with the position of the lifters, see Figs 5 and 6. This result gives a better insight to the grinding process and the travelling of the mechanical waves within the charge and mill lining. Within a grinding ball, the stress is distributed. To resolve that stress for each grinding ball in a mill is possible but very computationally costly and today not reasonable. Each ball has to contain a number of FE elements to resolve the stress field. To model grinding balls as single SPH particles give a constant stress. This means that the single SPH particle provides the mean value of the stress. The peak values will not be found with this approach but it will give an idea of how the global stress field looks like.

A combination of Figs. 4 to 6 reveals that the area with slow-moving grinding balls overlaps the areas with maximal internal charge pressure and shear stress. This is an important result, since this combination may be considered to maximise the attrition process that generates the fine particles in grinding. Being able to predict the extension of this area, and the magnitude of the stresses in it, opens up the possibility for improving the energy efficiency in tumbling mills.

The presented SPH-FEM model gives a physically accurate presentation of the system. The liner design has a large influence on the charge motion but the charge is also changed during its passage through the mill. Better description of the charge behaviour will help to optimise liner design. This may minimize energy consumption and increase the efficiency of the milling process.

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REFERENCES


NUMERICAL AND EXPERIMENTAL INVESTIGATION OF MIXING IN A CONTINUOUSLY OPERATED FLUIDIZED BED

HOLD J., WIRTZ S. AND SCHERER V.

Department of Energy Plant Technology
Ruhr-Universitaet Bochum
Universitaetsstr. 150, 44780 Bochum, Germany
e-mail: hold@leat.rub.de, www.leat.ruhr-uni-bochum.de/

Key words: Fluidized Bed, DEM, CFD, Euler-Euler Method.

Abstract. Many processes require solid material to be fed continuously into a fluidized bed. In order to study the related mixing process of the solid feed with the bed material, a laboratory scale experiment with a continuous supply system is set up and monitored with a high resolution camera system. Additionally, two simulation methods are used: The Euler-Euler and an Euler-Lagrange approach based on the Discrete-Element-Method (DEM) coupled with CFD. Experimental investigations carried out at varying fluid velocities are compared with simulations. A reasonable agreement is found between the coupled DEM-CFD-method and the experimental findings.

1 INTRODUCTION

Fluidized beds are widely used systems for a variety of processes involving particulate solids. These systems have many applications in engineering such as combustion, drying, granulation and coating. Many processes require a solid material to be conveyed into a fluidized bed, to remain a certain time within the bed and to be discharged afterwards. This can be done in batch operation, however for larger quantities continuous operation is more favorable. Since mixing is expected to be “fast” in technical systems, the actual time scales associated with the mixing process are usually unknown. In this context it is important to analyze how the imparted particular solid is mixed in the fluidized bed.

To investigate this process in detail a laboratory scale experiment with a continuous particle supply system is set up in which particle motion is monitored through a high resolution camera system. Additionally, two different simulation methods are applied. The first simulation method is the Euler-Euler-approach [1, 2] where both solids and fluid are modeled in the framework of the Navier-Stokes equations incorporating the kinetic theory of granular flow. In addition as second method the coupled CFD/Discrete-Element-Method (DEM) is used [3, 4] where the particles are modeled on the grain scale based on Newton’s and Euler’s equations while the fluid is considered as a continuum described by the Navier-Stokes equations. In the following the experimental setup and the applied simulation methods are briefly explained, initial results are presented and discussed.
2 EXPERIMENTAL SETUP

The laboratory scale fluidized bed has a square base and is made out of polycarbonate (110 x 110 x 400 mm³). A sketch is given in figure 1. The system is equally fluidized from the bottom through a porous plate at adjustable fluid velocities. The bed initially consists of d=7 mm spherical particles made out of polyoxymethylene (POM). The initial bed height without fluidization is 110 mm. Particles can be inserted into the fluidized bed through a supply system which is connected to the bed at a height of 34 mm above the ground plate. In the experiments performed, a solid mass flow of 7.67 g/s is introduced through this supply for 30 seconds. Particles are discharged from the system in a height of 175 mm through a drain channel. The particles inserted into the system are of smaller size (d=5 mm) and different color than the particles forming the initial bed. Further details on the particles in the bed and in the supply system are presented in table 1.

![Figure 1 Outline of the experimental setup](image)

Table 1: Details on the particles

<table>
<thead>
<tr>
<th></th>
<th>Particles in the bed</th>
<th>Particles in the supply system</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter</td>
<td>7 mm</td>
<td>5 mm</td>
</tr>
<tr>
<td>Density</td>
<td>1182.95 kg/m³</td>
<td>1182.95 kg/m³</td>
</tr>
<tr>
<td>Material</td>
<td>POM</td>
<td>POM</td>
</tr>
<tr>
<td>Number</td>
<td>4660</td>
<td>2970</td>
</tr>
<tr>
<td>Color</td>
<td>Blue (gray)</td>
<td>Yellow (white)</td>
</tr>
<tr>
<td>Mass Flow Rate</td>
<td>---</td>
<td>7.67 g/s (≈ 100 particles/s)</td>
</tr>
</tbody>
</table>

The particle motion is monitored through a high resolution camera system Motion Blitz 500 (Mikrotron). Differently coloured particles of varying sizes allow for a quantitative evaluation of mixing and composition within the fluidized bed and at the solid’s inlet and outlet.

3 MATHEMATICAL MODELLING

In addition to the experiments two different simulation methods are used and compared. Firstly, the Euler-Euler-framework is described followed by the Euler-Lagrange-method used
as second approach.

**A. EULER-EULER-MODEL**

The Euler-Euler-Method based on the work by Savage and Jeffrey [1] and Ding and Gidaspow [2] considers the fluid phase as well as the particle phases as a continuum. Derived quantities are averaged per cell. Particles with the same characteristics are pooled in different particle phases. The volume fractions of the particle phases together with the volume fraction of the fluid phase sum up as

\[
\varepsilon_F + \sum_{i=1}^{n_p} \varepsilon_{pi} = 1
\]

where \(\varepsilon_F \geq 0\) is the porosity of the fluid, \(n_p \in \mathbb{N}\) is the number of the particle phases and \(\varepsilon_{p1}, \ldots, \varepsilon_{pn_p} \geq 0\) are the volume fractions of the respective phases \(1, \ldots, n_p\). For any phase the equation of continuity applies. On the one hand the equation of continuity for the fluid phase is defined as

\[
\frac{\partial(\varepsilon_F \rho_F)}{\partial t} + \nabla(\varepsilon_F \rho_F \vec{v}_F) = \vec{0}
\]

where \(\rho_F\) is the density of the fluid and \(\vec{v}_F\) is the velocity-vector of the fluid. And on the other hand the equation of continuity for the particle phases is defined as

\[
\frac{\partial(\varepsilon_p \rho_p)}{\partial t} + \nabla(\varepsilon_p \rho_p \vec{v}_p) = \vec{0}
\]

for all phases \(1, \ldots, n_p\) where \(\rho_p\) is the density of the particles, \(\vec{v}_p\) is the velocity-vector of the particle phase and \(\varepsilon_p = 1 - \varepsilon_F\) for \(i=1, \ldots, n_p\) is the volume fraction of each particle phase considered per cell. Furthermore any phase has to achieve the balance of the momentum. For this purpose the tensor of the shear rate \(\bar{S}_F\) and the stress tensor \(\bar{\tau}_F\) for the fluid phase are given as

\[
\bar{S}_F = \frac{1}{2} [\nabla \vec{v}_F + (\nabla \vec{v}_F)^T] - \frac{1}{3} \nabla \vec{v}_F \bar{I},
\]

\[
\bar{\tau}_F = 2\varepsilon_F \mu_F \bar{S}_F.
\]

Analogical the required tensor of the shear rate \(\bar{S}_p\) and the stress tensor \(\bar{\tau}_p\) for the particle phases are defined as

\[
\bar{S}_p = \frac{1}{2} [\nabla \vec{v}_p + (\nabla \vec{v}_p)^T] - \frac{1}{3} \nabla \vec{v}_p \bar{I},
\]

\[
\bar{\tau}_p = 2\varepsilon_p \mu_p \bar{S}_p.
\]
The equation of momentum for the fluid phase which interacts with \(n_p\) phases of particles, reads

\[
\frac{\partial (\varepsilon_f \rho_f \vec{v}_f)}{\partial t} + \nabla \left( \varepsilon_f \rho_f \vec{v}_f \right) = \nabla (\varepsilon_f \rho_f \vec{g}) + \varepsilon_f \rho_f \vec{g} - \varepsilon_f \rho_f \nabla p + \sum_{i=1}^{n_p} \beta_i (\vec{v}_i - \vec{v}_p) \tag{8}
\]

where \(\vec{g}\) is the acceleration of gravity, \(\nabla p\) is the pressure gradient and \(\beta\) is the drag coefficient representing the inter-phase momentum exchange, which is described below. The drag coefficient distinguishes between \(\varepsilon_f \leq 0.8\) and \(\varepsilon_f > 0.8\) according to Gidaspow and Ding [2]:

\[
\beta_i = \begin{cases} 
150 \left(1 - \varepsilon_f\right)^2 \frac{\mu_f}{d_p} + 1.75 \left(1 - \varepsilon_f\right) \frac{\rho_f d_p}{d_p} | \vec{v}_f - \vec{v}_p | & \text{for } \varepsilon_f \leq 0.8 \quad [5] \\
3 \rho_f C_d \left(1 - \varepsilon_f\right) \varepsilon_f^{-4.7} \frac{d_p}{d_p} | \vec{v}_f - \vec{v}_p | & \text{for } \varepsilon_f > 0.8 \quad [6]
\end{cases}
\tag{9}
\]

for any phases \(i = 1, \ldots, n_p\) where \(d_p\) is the considered particle diameter, \(\mu_f\) is the characteristically dynamic viscosity of the fluid and

\[
C_d = \begin{cases} 
24 \left[1 + 0.15 (\text{Re}_p)^{0.587}\right] & \text{for } \text{Re}_p < 1000 \quad [6] \\
0.44 & \text{for } \text{Re}_p \geq 1000 \quad [6]
\end{cases}
\tag{10}
\]

with

\[
\text{Re}_p = \frac{\varepsilon_f \rho_f | \vec{v}_f - \vec{v}_p | d_p}{\mu_f}.
\tag{11}
\]

The equation of momentum for the particle phase \(j\) and its interaction with the fluid phase and \((n_p - 1)\) particle phases \((n_p > 0)\) is defined as

\[
\frac{\partial (\varepsilon_j \rho_p \vec{v}_j)}{\partial t} + \nabla (\varepsilon_j \rho_p \vec{v}_j) = \nabla (\varepsilon_j \rho_p \vec{g}) + \varepsilon_j \rho_p \vec{g} - \varepsilon_j \rho_p \nabla p_j + \beta_j (\vec{v}_j - \vec{v}_p) + \sum_{i=1}^{n_p-1} \beta_i (\vec{v}_j - \vec{v}_p) \tag{12}
\]

in which \(\varepsilon_j\) is the volume fraction, \(\vec{v}_j\) is the velocity-vector, \(\tau_j\) is the stress tensor, \(\nabla p_j\) is the pressure gradient, \(\beta_j\) is the drag coefficient of the particle phase \(j\). Using the kinetic theory of granular flow the pressure and the viscosity of the particle phases are calculated. Further details can be found in [2, 7].

**B. Euler-Lagrange-Model**

In the Euler-Lagrange-Model the particle motion is described by a three-dimensional soft-sphere Discrete-Element-Method (DEM). The mechanical behavior of the particles is calculated by integration of the Newton and Euler equations of motion. Thus, the positions and the translational and rotational velocities can be calculated for any particle in the bed.
The force \( \vec{F}_i \), which affects a particle \( i \), is given by

\[
\vec{F}_i = m_i \ddot{\vec{a}}_i(t) = \vec{F}_{G,i} + \vec{F}_{D,i} + V_i \nabla p_i + \sum_{j=1}^{n} \vec{F}_{pw,j,i} + \sum_{j=1}^{n} \vec{F}_{pf,j,i},
\]

where \( \ddot{\vec{a}}_i(t) \) is the acceleration and \( m_i \) is the mass of a particle \( i \), \( \vec{F}_{G,i} = m_i \vec{g} \) is the gravitational force, \( \vec{F}_{D,i} = -\beta_i (\bar{v}_{pi} - \bar{v}_F) \) is the drag forces, which results from the relative difference of fluid and averaged particle velocities, \( V_i \) is the volume of a particle \( i \), \( \nabla p_i = -\beta_i (\bar{v}_{pi} - \bar{v}_F) / \varepsilon_F \) is the pressure gradient leading to a pressure gradient force and \( \vec{F}_{pw,j,i} \) are the contact forces resulting from the interaction with other particles or walls. Rotational motion of a particle \( i \) is given by

\[
\vec{M}_i = J_i \frac{d\vec{\omega}_i}{dt} = \sum_{j=1}^{n} \vec{M}_{ij},
\]

where \( \vec{M}_{ij} \) are the external moments acting on the particle, \( \vec{\omega}_i \) is the angular velocity and \( J_i \) is the moment of inertia. The interaction between the particles is calculated using a soft-sphere-method, which is based on linear spring-damper models [8, 9].

The fluid phase is modeled by a Computational Fluid Dynamics (CFD) tool. The coupled continuity and momentum equations are solved defined as

\[
\frac{\partial (\varepsilon_F \rho_F)}{\partial t} + \nabla (\varepsilon_F \rho_F \bar{v}_F) = 0,
\]

\[
\frac{\partial (\varepsilon_F \rho_F \bar{v}_F)}{\partial t} + \nabla (\varepsilon_F \rho_F \bar{v}_F \bar{v}_F) = \nabla (\varepsilon_F \bar{\tau}_F) - \varepsilon_F \nabla \bar{p} + \varepsilon_F \rho_F \bar{g} + \vec{f}_{int}.
\]

The vector \( \vec{f}_{int} \) describes the change of the momentum which results from the interaction between the fluid and the particles.

However, instead of solving equations (15) and (16) directly e.g. [3, 4], (15) and (16) can be transformed by rules of differential calculus [10] into

\[
\frac{\partial (\rho_F)}{\partial t} + \nabla (\rho_F \bar{v}_F) = -\rho_F \left( \frac{\partial \varepsilon_F}{\partial t} + \bar{v}_F \nabla \varepsilon_F \right),
\]

\[
\frac{\partial (\rho_F \bar{v}_F)}{\partial t} + \nabla (\rho_F \bar{v}_F \bar{v}_F) = \bar{\tau}_F - \nabla \bar{p} + \rho_F \bar{g} + S_m.
\]

with \( S_m = \frac{\vec{f}_{int}}{\varepsilon_F} + \frac{\bar{\tau}_F}{\varepsilon_F} \nabla \varepsilon_F - \rho_F \left( \frac{\partial \varepsilon_F}{\partial t} + \bar{v}_F \nabla \varepsilon_F \right) \bar{v}_F \).
On the left side of the equal signs the classical single phase continuity and momentum equations can be identified. The solution of (17) and (18) allows for a faster convergence and therefore faster simulations especially if the momentum source terms $\mathbf{f}_{\text{int}}$ are further linearized by the fluid velocity [10].

4 RESULTS AND DISCUSSION

For this paper results from two different simulation methods are compared to experimental findings for two different superficial velocities which are larger than the minimal fluidization velocity of the initial bed of $v=2$ m/s. It is expected that the particles introduced through the supply system mix faster with the particles in the bed if the superficial velocity is chosen larger.

In figure 2 results for the Euler-Euler-Method after 15 s are shown. When comparing the two cases with superficial velocities of 2.3 m/s and 2.8 m/s it is hardly possible to recognize differences in the spatial distribution of the volume fraction introduced by the feed stream. The distribution within the bed is very similar.

As could be concluded from figure 2, an assessment of the mixing behavior of different particle phases at varying fluid velocities, using the Euler-Euler-Method offers no detailed insight especially for the relatively large particle considered here.

In the following figures results from the experiments (figure 3) and from the coupled CFD-DEM-simulations (figure 4) are shown. In both figures it can be observed that at larger fluid velocities (leading to increased particle motion) the mixing is positively affected. In contrast, at the smaller superficial velocity of 2.3 m/s only few particles from the supply system can be seen on the periphery of the bed.
On the left side of the equal sign the classical single phase continuity and momentum equations can be identified. The solution of (17) and (18) allows for a faster convergence and therefore faster simulations especially if the momentum source terms $\int \rho \ \mathbf{f} \ \mathbf{a}$ are further linearized by the fluid velocity [10].

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In order to analyze the mixing behavior quantitatively, the variance $s_m^2$ is used:

$$s_m^2 = \frac{1}{m} \sum_{i=1}^{m} (X_i - P)^2,$$

where $m$ is the number of spot tests, $X$ is the actual concentration and $P$ is the ideal concentration. Because of the dynamics of the system, the ideal concentration changes with time and is dependent on the feed mass flow.

The variances calculated from the simulations and the experiments confirm the previous results (figure 5). After 15s the variance at the superficial velocity of 2.3 m/s is clearly larger than at a superficial velocity of 2.8 m/s in experiment and simulations. At a larger fluid velocity the particles experience more fluctuations therefore mixing can occur more easily and the variance can thereby decrease. In figures 5d and 5f the variance is presented for the experiment and the Euler-Lagrange-Method at a velocity of 2.8 m/s. Both graphs indicate certain fluctuations in the variance in contrast to the lower velocity of 2.3 m/s. In the Euler-Euler-Method these fluctuation cannot be observed. The fluctuations of the variance are an effect of the particle motion on the micro scale and therefore cannot be observed in the Euler-Euler-method. Differences exist between the overall levels of the variance in the coupled CFD-/DEM-Method and in the experiment. Further effort has to be put into ensuring that conditions in the experiment and simulations are equal.
5 CONCLUSIONS
The mixing behavior of a particle feed into a fluidized bed was investigated at different superficial velocities. For this purpose a laboratory scale experiment was set up. Additionally, two different simulation methods were utilized. On the one hand the Euler-Euler-Method, which describes all phases as continuum, was used and on the other hand an Euler-Lagrange-Method, which describes the particles in a discrete way combined with a continuum description for the fluid phase, was applied.

The results show that in the Euler-Euler-Method the superficial velocity has only a minor influence on the mixing behavior. In contrast, the experiment and the Euler-Lagrange-Method reveal that in case of an increased fluid velocity mixing is amplified. It can be concluded that the Euler-Euler-method is of limited applicability to mixing processes of particles of the size studied here. For the future the alignment between the experiment and the simulations has to be further improved to allow for a quantitative comparison.
REFERENCES


COSIMULATION OF MBD (MULTI BODY DYNAMICS) AND DEM OF MANY SPHERES USING GPU TECHNOLOGY

JOON SHIK YOON *, JI SOO PARK †, CHEOL O AHN †† AND JIN HWAN CHOI †

*Department of Mechanical Engineering
Seoul National University
Seoul 151-742, Korea
e-mail: jueno@functionbay.co.kr

† Department of Mechanical Engineering
Kyung Hee University
Yongin 449-791, Korea
e-mail: jspark83@functionbay.co.kr, jhchoi@khu.ac.kr

†† Metariver Technology Co., Ltd.
Seongnam 463-841, Korea
e-mail: coahn@metariver.kr

Key words: MBD, DEM, Particle Dynamics, Cosimulation

Abstract. In this paper, dynamic simulation model which have many sphere particles and MBD (Multi Body Dynamics) entities, i.e. bodies, joints, forces, is built and simulated. Many sphere particles are solved with DEM (Discrete Element Method) and simulated with GPU technology. Fast algorithm is applied to calculate hertzian contact forces between many sphere particles (from 100,000 to 1,000,000) and NVIDIA’s CUDA is used to accelerate the calculation. Explicit integration method is applied to solve the many spheres. MBD (Multi Body Dynamics) entities are simulated with recursive formulation. Constraints are reduced by recursive formulation and implicit generalized alpha method is applied to solve dynamic model. Many sphere particles and MBD (Multi Body Dynamics) entities are co-simulated within commercial software RecurDyn. The interaction forces between many sphere particles and rigid body mesh are calculated and applied to each body to simulate two parts simultaneously. These models are built and simulated; fork lifter with sand model, oil in oil tank model, oil filled engine system and water filled washing machine model. All models are simulated with NVIDIA’s GPU and the result is shown.
1 INTRODUCTION

Today, parallel GPUs have begun making computational inroads against the CPU and general purpose GPU can be used in simulation algorithm to amplify the performance. The parallel implementation of algorithm, when executed on a ubiquitous Graphics Processing Unit (GPU) card, yields a 30 fold speedup over a similar algorithm executed on the Central Processing Unit (CPU). With the introduction of NVIDIA’s Compute Unified Device Architecture (CUDA) [1], GPUs are now able to run C code natively on the device instead of relying on interpreted code.

A discrete element method (DEM) is any of family of numerical methods for computing the motion of a large number of particles of micrometre-scale size and above. As GPU can boost the calculation speed of parallel programming, DEM (Discrete Element Method) is becoming widely used in granular and discontinuous materials, especially in granular flows, powder mechanics, and rock mechanics. Some examples are granular matter (rock, sand, soil), powders, liquid and solutions. And typical industries using DEM are chemical, pharmaceutical, mining, agriculture and food handling, powder metallurgy and digital printing. With advances in computing power and numerical algorithms, it has become possible to simulate millions of particles numerically.

While many particles are solvable with DEM and parallel programming, it is called Particle Dynamics in this study; the only Particle Dynamics have a limitation on system modeling which can cover system with constraints and motions. Whole dynamic simulation mostly handle constraints and motions and even can be connected with other technique like control, optimization. RecurDyn[2] is commercial software and simulates multi body dynamics and finite element together. If the particle dynamics is included in MBD, the synergy effect of the simulation can be enlarged.

To connect two kinds of the simulation, MBD and Particle Dynamics, the dividing domain algorithm and interaction algorithm is essential. Within these algorithms, the cosimulation should be performed well even though two simulations are quite different. In this study, cosimulation of MBD and Particle Dynamics is introduced and the algorithms of dividing and interaction are also explained.

This paper is organized as follows. After introduction basic theories of Particle Dynamics on DEM and MBD are shown in charter 2.1 and 2.2 respectively. Integration methods of each method are described in chapter 2.3. Cosimulation of two methods is given in chapter 2.4. and GPU acceleration technique is given in chapter 2.5. Chapter 3 is numerical experiment for Particle Dynamics validation. Chapter 4 is cosimulation of Particle Dynamics and MBD. Final chapter summarize the conclusion of this study.

2 FORMULATION

2.1 PARTICLE DYNAMICS (DEM)

Particle-based techniques are used in many applications. DEM is a numerical method for computing the behavior of large number of solid-particle system. This simulation method consists of the idea of determining the kinematic force to each finite-sized particle. All forces acting on each particle are modeled and calculated at every discrete-time step.[3][4] In time
integration algorithm, most of the MBD solvers are using implicit algorithm but DEM adopts explicit time-integration. The trajectories of particles are updated by Newton’s law of motion, according to the following equations:

\[
\frac{dv}{dt} = \sum \frac{F}{m} \tag{1}
\]

\[
\frac{d\omega}{dt} = \sum \frac{M}{I} \tag{2}
\]

where \(v\) is the particle velocity, \(F\) is the summed force acting on a particle, \(m\) means the mass of a particle, \(\omega\) is the angular velocity, and \(M\) and \(I\) denote the moment of force and the moment of inertia.

A contact model between two particles is given by the Hertzian contact model and Voigt model, which consists of a spring dashpot and a slider for the friction in the tangential component\[5\]. The contact forces \(F_n\), compressive, and \(F_t\), shear, are calculated by the following equations:

\[
F_{n,ij} = k_n |\Delta|^{0.5} n_{ij} + c_n u_{n,ij} |\Delta|^{0.25} \tag{3}
\]

\[
F_{t,ij} = \min\left[k_t |\Delta|^{0.5} t_{ij} + c_t u_{t,ij} |\Delta|^{0.25}, \mu_j |F_n| t_{ij}\right] \tag{4}
\]

where \(k\) and \(c\) designate the spring and the damping coefficients, the vectors \(n_{ij}\) and \(t_{ij}\) are the unit vectors from the \(i\)-th particle to the \(j\)-th one in normal and tangential components, \(\Delta\) and \(u\) are the deformation by contact and relative velocity of two particles, respectively.

The force acting on a body can be obtained from the particles which contact on the body by summing their force.

### 2.2 Multi Body Dynamics (MBD)

Rigid body dynamics can be modeled using various formulations (Jalón and Bayo \[6\]). In this investigation, the recursive formulation is used. This section provides an introduction to the recursive formulation. The coordinate systems for two contiguous rigid bodies in 3D space are shown in Fig. 1. The two rigid bodies are connected by a joint, and an external force \(F\) is acting on the rigid body \(j\). The X-Y-Z frame is the inertial or global reference frame and the \(x'-y'-z'\) is the body reference frame with respect to the X-Y-Z frame. The subscript \(i\) means the inboard body of body \(j\) in the spanning tree of a recursive formulation (Bae et al. 2001)\[7\].
The equations of motion for a constrained mechanical system (García de Jalón et al. [8]) in the joint space (Wittenburg [9]) are then obtained by using the velocity transformation method as follows:

$$F = B^T(M\dot{Y} + \Phi^T\lambda - Q) = 0$$  \hspace{1cm} (5)

where $\Phi$ and $\lambda$, respectively, denote the cut joint constraint and the corresponding Lagrange multiplier. $M$ is a mass matrix and $Q$ is a force vector including the external forces in the Cartesian space.

### 2.3 Implicit and Explicit Integrator

For the multibody systems, there are various methods of implicit and explicit solution procedures that are used to solve the semi-discrete equations of motion along with the constraint. In implicit solution procedure, a solution for the system displacements that simultaneously satisfies the equations of motion and constraints is sought at each time step given the solution at the previous time step. Since the equations are nonlinear, Newton-Raphson equilibrium iterations are performed to guarantee that an equilibrium solution is reached at each time step (Brenan et al. [10], Haug and Deyo [11], Hairer and Wanner [12]). Implicit solution procedures are unconditionally stable. However, the time step should be at least an order of magnitude smaller than the smallest natural period that needs to be resolved. An advantage of implicit solution procedures over explicit procedures is that the time step can be much larger than the smallest natural period of the system, which can be very small for very stiff systems. There is a very close relationship between the solution methods and the constraints modeling methods. The floating frame approach is usually used in conjunction with the Lagrange multiplier method for imposing the constraints.

In explicit solution procedures (Hughes and Belytschko [13]), a solution for the accelerations that satisfies the equations of motion and constraints is sought at each time step. If a mass matrix is used, then the system’s equations of motion are uncoupled at each time step and they can be directly solved for the accelerations. A typical explicit algorithm starts by evaluating the vector of internal forces from the known positions and velocities at time step $t$. Then, internal forces are added to the external forces. The equations of motion are then directly used to calculate the accelerations at time step $t + \Delta t$. A time integration formula
such as the trapezoidal rule is used to integrate the acceleration into the velocities and positions at time step $t + \Delta t$.

Explicit temporal integration techniques are only conditionally stable because the time step must be smaller than the equation’s characteristic time. If the same time step is used for the entire system, then that time step must be smaller than the smallest natural period of all bodies. This imposes a severe time step restriction and generally means that a very large number of time steps are needed to obtain the dynamic response.

Multi body dynamics have constraints and therefore constraints are satisfied with implicit integration. The governing equations of multibody dynamics, which are derived previous sections, is solved using the implicit generalized-alpha method (Chung and Hulbert [14]), which has a nonlinear stepping equation. By the way particles are have huge DOF compared with MBD and there are no constraint equations. The particles are solved with explicit integration and it is accelerated with parallel processing using GPU.

2.4 Cosimulation of Particle Dynamics and MBD

Simulation of many particles in multi body systems needs strategy of cosimulation. Many particles are solved with explicit integration and multi body systems are solved with implicit integratioon. Figure 2 shows a sample idea of cosimulation about MBD and particles. The whole modeling is composed with a spring, a box and many spheres. The spring and the box is solved with RecurDyn[2](MBD Solver) while many particles are solved with SAMADII\textsuperscript{TM}[15] (Particle Solver). Two solver divides the model with boundaries and in this sample the box is the boundary. The boundary force is given by the Particle Solver and boundary position, velocity is given by the MBD Solver.

Figure 2. Modeling of MBD and Particle Dynamics
2.5 Simulation Acceleration Techniques (GPU)

The main disadvantage of particle-based simulation with a very large number of particles is that it requires a very heavy computing resources to obtain satisfactory results. But it is relatively not so difficult to parallelize particle systems. Perhaps GPU computing is the best way to achieve ability to handle large number of particle system efficiently.

Therefore we adopted the DEM solver using GPU system, the SAMADII™ (Metariver Technology co., ltd.) [15]. It was developed to simulate particle-based system using GPU.

GPUs are massively parallel multithreaded devices capable of executing a large amount of active threads. GPU has multiple streaming multiprocessors, each of which contains multiple scalar processor cores. A function that executes on the GPU consists of multiple threads executing code in a single instruction, multiple data (SIMD) fashion. That is, each thread in a kernel executes the same code, but on different data. The libraries CUDA from NVIDIA allows one to use the streaming microprocessors mounted in high-end graphics cards as general-purpose computing hardware. Presently, the raw computational power of these multiprocessors can reach one Teraflop, which is several hundred times the throughput of a modern scalar CPU.

The SAMADII™ was developed with hardware acceleration by GPU as well as software acceleration using the cell-linked list algorithm to accelerate DEM simulation.[16] The simulation space is partitioned into cells and the particles are then assigned to the cells so that it is easier to find the neighbors of a given particle. At the beginning of a simulation, an array that contains a list of cell neighbors for each cell is created. This method dramatically reduces the number of unnecessary inter-particle distance calculations.

3 PARTICLE DYNAMICS VALIDATION

A validation model is total weight of spheres in a box. 1,331 spheres are filled in a box as Figure 3. The weight of the sphere is 12.62kg and therefore the total weight of the spheres are 16797.22kg. And as a result of the simulation, the force imposed to the box by many spheres is 16765.38kg and there are only 0.19% error in weight of the total weight of the spheres.

![Figure 3. Total sphere weight in a box model](image-url)
4 COSIMULATION NUMERICAL EXPERIMENT

In this section simulation result of a cosimulation model is shown. The model is modeled in MBD software RecurDyn and the particles are cosimulated by SAMADI™. Figure 4 shows a waterfall model. The left figure is modeling of the waterfall and the other figures are simulation results of the spheres.

The model is simulated with one GPU TESLA2050 for many spheres. Table 1 listed the specification of the models; number of spheres, simulation time, stepsize, CPU time and so on.

Table 1. Result of cosimulation models

<table>
<thead>
<tr>
<th></th>
<th>Waterfall</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of spheres</td>
<td>52,000</td>
</tr>
<tr>
<td>Radius of spheres</td>
<td>0.01m</td>
</tr>
<tr>
<td>Simulation endtime</td>
<td>2 sec</td>
</tr>
<tr>
<td>Stepsize of MBD</td>
<td>1.0e-3</td>
</tr>
<tr>
<td>Stepsize of Particle</td>
<td>2.89e-6</td>
</tr>
<tr>
<td>CPU time</td>
<td>5 hour 51 mim</td>
</tr>
</tbody>
</table>

5 CONCLUSIONS

In this study Particle Dynamics is introduced which have high performance using GPU technology. And cosimulation of MBD and Particle Dynamics is also explained with connecting algorithm. The Particle Dynamics is validated with total sphere weight model. For the cosimulation result, waterfall model is modeled and simulated.

REFERENCES


MULTIBODY CONTACT DYNAMICS WITH COROTATIONAL FINITE ELEMENTS AND ROUGH BACKGROUND MESH

TOMASZ KOZIARA, ŁUKASZ KACZMARCZYK AND NENAD BIĆANIĆ

School of Engineering
University of Glasgow, Glasgow G12 8LT, UK
e-mail: t.koziara@civil.gla.ac.uk

Key words: co-rotational, FEM, simplified deformations, Contact Dynamics

Abstract. In this work we demonstrate a simple kinematic model allowing for a variable amount of deformability for arbitrary shapes. A co-rotational finite element formulation is integrated over a shape submerged in a rough background mesh. The presented formulation allows to approximate the structural length-scale shock waves within a multi-body structure, which might be seen as a refinement of the solely rigid approach, for which such resolution is not readily available. For best illustration of core ideas, only simple one-body examples are given in the current paper. Nevertheless, the kinematic model has been employed within the Contact Dynamics time-stepping method and applied to large scale, parallel simulations of blocky structures with contact and friction. The source code is available at http://solfec.googlecode.com.

1 INTRODUCTION

Rigid kinematics is commonly used in industrial multibody simulations (e.g. robotics or granular flow). This level of kinematic description is often sufficient when dynamic effects corresponding to the collective deformable behavior of bodies can be neglected. Whenever this is not the case though, a modeler often runs into problems with the computational bottleneck of processing many interacting bodies, discretised with fine Finite Element meshes. Because in the classical formulation mesh and shape coincide, small features of the shape may result in the necessity of resolving deformation length scales that might not be of practical interest in the overall collective behavior of large multibody problems. In order to facilitate this level of modeling, a simple extension of the classical Finite Element approach has been implemented in Solfec [5]: shapes and FE meshes can be prescribed independently. This is pictured in Figure 1, where a geometrical model of a complex shape is contained inside of background FE mesh with 96 nodes. In a multibody model of
a practical interest many thousands of such bodies interact through contact and friction. Clearly, it would be computationally difficult to resolve this kind of collective geometry by means of a fine, matching FE mesh.

Using the background mesh is only a simple, technical idea. The core contribution of this paper is the co-rotational Finite Element formulation, which allows to apply deformability at a very low cost. We adapt the work of Kaczmarczyk et al. [4] and design a simple body-wise co-rotational formulation, for which the global stiffness matrix is assembled and inverted only once. The subsequent linear solves only reuse a once computed factorization, while still being able to correctly account for large rigid rotations. Our approach is well suited for stiff, deformable bodies whose gross rigid motion is of engineering interest and whose deformability plays some role in a collective multibody dynamics. To this end we use stiffness-proportional damping, which does not affect the rigid motion, but which allows to model a range of post-impact behavior in an energy consistent, dissipative manner. Modeling multiple impacts and shock waves within a solely rigid, implicit multibody formulation is not possible in general, hence our approach provides a relatively inexpensive refinement in this respect.

2 ROTATED DYNAMICS

Consider a stiff body capable of large rigid motion and small elastic deformations. We can parametrize its motion as

$$\mathbf{x}(\mathbf{X}, t) = \mathbf{X} + \mathbf{S}(\mathbf{X}) \mathbf{q}(t) \quad (1)$$

where $\mathbf{x}$ is a spatial point, $\mathbf{X}$ is a referential point, $t$ is time, $\mathbf{S}$ stores finite element shape functions, and $\mathbf{q}$ stores nodal displacements. Because we consider infinitesimal deformations about a possibly translated and rotated shape, it makes sense to talk about the gross rigid motion.
\[ x_r (X, t) = \Lambda (t) (X - A) + a (t) \]  

(2)

where \( \Lambda \) is a rotation operator, \( A \) is a referential point, and \( a \) is a spatial image of \( A \). These two motions differ by the amount of deformation

\[ d (X, t) = x (X, t) - x_r (X, t) \]  

(3)

Assuming that \( Z_i \) are coordinates of mesh nodes, we can collect \( d (Z_i, t) \) into a vector

\[ d = \begin{bmatrix} Z_i + q_i - \Lambda (Z_i - A) - a \\ ... \\ ... \end{bmatrix} \]  

(4)

where \( q_i \) represent displacements at node \( i \). We can also express \( d \) from the perspective of the reference configuration

\[ d_0 = \Lambda^T d \]  

(5)

where \( \Lambda \) denotes a block-diagonal square matrix composed of \( \Lambda \) and matching the dimension of \( d \). We can then write down a discrete form of momentum conservation

\[ M \dot{d} u + \Delta K \Delta^T (d dt + \eta u dt) = f dt \]  

(6)

where \( M \) is a mass matrix, \( du \) and \( dt \) are suitable velocity and time measures, \( K \) is an initial stiffness matrix \( K = \partial^2 \Psi / \partial \dot{q} \partial \dot{q} \) at \( t = 0 \) where \( \Psi \) is a hyper-elastic potential, and \( f \) is an external force. We note, that the term \( \eta \Delta K \Delta^T u \) corresponds to a stiffness-proportional damping, which can be used to damp out fast elastic oscillations without affecting the rigid body motion. At this point it is useful to notice that \( A \) and \( a \) in (4) play no role in (6) since rigid translations correspond to zero eigenvalues of \( K \). Hence, we can redefine \( d \) as

\[ d = \begin{bmatrix} (I - \Lambda) Z_i + q_i \\ ... \\ ... \end{bmatrix} = (I - \Lambda) Z + q \]  

(7)

where \( I \) is the \( 3 \times 3 \) identity. This corresponds to the deformation

\[ d (X, t) = x (X, t) - \Lambda (t) X \]  

(8)

which superposes rigid translation and small deformations of the body. As a result symmetric part of gradient of (8) equals to the symmetric part of the gradient of (3). This fact will be used in Section 4.
3 TIME INTEGRATION

Consider a multi-body domain with constraints. Let the constraint reactions be denoted by \( R \) and the relative constraints velocities be denoted by \( U \). Let also the constraints equations be denoted by \( C (U, R) = 0 \). When talking about \( q, u, \Lambda, \) etc. we now mean suitable collections of per-body entities. In order to integrate in time, a half-step configuration is extrapolated first

\[
q^{t+h/2} = q' + \frac{h}{2} u'
\]  
(9)

\[
\Lambda_1 = \dot{\Lambda} \left( q^{t+h/2}, \Lambda' \right).
\]  
(10)

A global \( u \) to local \( U \) velocity transformation operator is computed next

\[
H = H \left( q^{t+h/2} \right)
\]  
(11)

where for example, in case of Finite Elements, \( H \) is a global to local coordinates transformation of the shape functions values nonzero at constraint points. The number of rows of \( H \) depends on the number of constraints, while its rank is related to their linear independence. The momentum balance

\[
b = Mu' + hf^{t+h/2} - h\Lambda_1 K \Lambda_1^T \left[ \left( I - \Lambda_1 \right) Z + q^{t+h/2} + \eta u' \right]
\]  
(12)

\[
\left( M + \frac{h^2}{4} \Lambda_1 K \Lambda_1^T \right) u^{t+h} = b + H^T R
\]  
(13)

together with the transformation

\[
U = Hu^{t+h}
\]  
(14)

and the constraints equations

\[
C (U, R) = 0
\]  
(15)

are used to evaluate the velocity \( u^{t+h} \) and the constraint reactions \( R \). This is further commented on in Section 5. For the sake of simplicity the term \( \eta u' \) is explicit in (12). The stiffness-proportional damping is a pragmatic, numerical device here: we use to avoid uninteresting oscillations and to drive post-impact behavior. Finally, the end-step configuration is updated

\[
q^{t+h} = q^{t+h/2} + \frac{h}{2} u^{t+h}
\]  
(16)

\[
\Lambda^{t+h} = \dot{\Lambda} \left( q^{t+h}, \Lambda_1 \right).
\]  
(17)
The above scheme is linearly-implicit: as far as unconstrained motion is concerned only one linear system needs to be solved per time step. A fully implicit version of the time integration scheme will be presented in a longer version of the article.

4 UPDATE ROTATION

Kaczmarczyk et al. [4] developed a convenient way of updating rotation, as needed in (10), and (17). Because the antisymmetric part of the gradient of the deformational displacement (8) corresponds to an infinitesimal rotation at a point, an average of it

$$\nabla \dot{d} = \frac{1}{V} \int_{\Omega} \nabla d(X, t) - \nabla d^T(X, t) \, d\Omega$$

(18)

represents the resultant infinitesimal rotation of the body (V is the volume). For every d, Λ is incremented in such a way so to minimise \(\nabla \dot{d}\). The divergence theorem is exploited in [4] in order to obtain

$$\text{vec} \left[ \int_{\Omega} \nabla d - \nabla d^T d\Omega \right] = \int_{\Gamma} n \times d d\Gamma$$

(19)

where vec[·] makes a pseudo-vector out of an antisymmetric matrix, and n is the spatial outward normal to the surface of the body. The surface integral can be further resolved

$$h = \int_{\Gamma} n \times d d\Gamma = \int_{\Gamma} \text{skew}[n] d d\Gamma$$

$$= \int_{\Gamma} \text{skew}[\Lambda N] d d\Gamma = \int_{\Gamma} \text{skew}[N] \Lambda^T d d\Gamma$$

$$= \int_{\Gamma} \text{skew}[N] \Lambda^T [X + S(X) q - \Lambda X] d\Gamma$$

$$= \int_{\Gamma} \text{skew}[N] \Lambda^T x d\Gamma$$

(20)

where the simplification to the last line follows from the assumption \(\int_{\Gamma} f d\Gamma \simeq \int_{\Gamma_0} f d\Gamma_0\) and the fact that \(\int_{\Gamma} \text{skew}[N] X d\Gamma = \text{vec} \left[ \int_{\Omega} \nabla X - \nabla X^T d\Omega \right] = 0\). The operator skew[·] makes a skew symmetric matrix out of a vector so that skew[n] d = n × d. The following functional is then defined

$$J(q, \Lambda) = \frac{1}{2} h^T(q, \Lambda) h(q, \Lambda)$$

(21)

and the \(\hat{\Lambda}\) mapping employed in the previous section takes form

$$\hat{\Lambda}(q, \Lambda) = \exp(\Phi) \Lambda, \text{ where } \Phi = \arg \min J(q, \exp(\Phi) \Lambda)$$

(22)
where \( \exp \) is the exponential map. Gauss-Newton iterations are exploited in order to compute the minimiser

\[
\Phi^{i+1} = \Phi^i - \{ \partial^2 J / \partial \Phi \partial \Phi \}^{-1} \{ \partial J / \partial \Phi \} \tag{23}
\]

where

\[
\begin{align*}
\partial J / \partial \Phi &= \mathbf{h}^T [\partial \mathbf{h} / \partial \Phi] \\
&= \mathbf{h}^T \left[ \int_{\Gamma} \text{skew} [\mathbf{N}] \Lambda T \frac{\partial \exp (\Phi)}{\partial \Phi} x d\Gamma \right] \\
\partial^2 J / \partial \Phi \partial \Phi &= [\partial \mathbf{h} / \partial \Phi]^T [\partial \mathbf{h} / \partial \Phi] + \mathbf{h}^T [\partial^2 \mathbf{h} / \partial \Phi \partial \Phi] \\
&\simeq [\partial \mathbf{h} / \partial \Phi]^T [\partial \mathbf{h} / \partial \Phi] + \delta \mathbf{I} \tag{25}
\end{align*}
\]

and \( \delta \) is large enough to make \( \partial^2 J / \partial \Phi \partial \Phi \) positive definite, ensuring a descent direction in (23). In practice, for this \( 3 \times 3 \) problem, \( \delta = 0 \) works well.

5 HANDLING CONSTRAINTS

Let

\[
\mathbf{A} = \mathbf{M} + \frac{\mathbf{h}^2}{4} \Lambda_1 \mathbf{K} \Lambda_1^T, \tag{26}
\]

In order to compute the constraints reactions we need to solve the nonlinear system

\[
\mathbf{A} \mathbf{u}^{t+h} = \mathbf{b} + \mathbf{H}^T \mathbf{R} \tag{27}
\]

\[
\mathbf{U} = \mathbf{H} \mathbf{u}^{t+h} \tag{28}
\]

\[
\mathbf{C} (\mathbf{U}, \mathbf{R}) = 0. \tag{29}
\]

An important aspect in this context is inversion of \( \mathbf{A} \). For a diagonal (lumped) \( \mathbf{M} \) (with constant per-node values) there holds

\[
\mathbf{A} = \Lambda_1 \left[ \mathbf{M} + \frac{\mathbf{h}^2}{4} \mathbf{K} \right] \Lambda_1^T = \Lambda_1 \mathbf{A}_0 \Lambda_1^T \tag{30}
\]

and it follows

\[
\mathbf{A}^{-1} = \left[ \Lambda_1 \mathbf{A}_0 \Lambda_1^T \right]^{-1} = \Lambda_1 \left[ \Lambda_1 \mathbf{A}_0 \right]^{-1} = \Lambda_1 \mathbf{A}_0^{-1} \Lambda_1^T \tag{31}
\]

so that it is enough to invert \( \mathbf{A}_0 \) only once.
A variety of constraints can be described in the form (29). These include contact, friction and a range of common equality constraints. An example of solving the system (27-29) in case of frictional contact constraints can be found in [3, 5], while a broader overview can be found in [2, 1].

6 ROUGH BACKGROUND MESH

A geometrical model of a complex shape, contained inside of background FE mesh with 96 nodes is presented in Figure 1. The technicalities of the background mesh approach are quite straightforward. The background mesh needs to properly contain the modeled shape. Since the Finite Element shape functions are partition of unity regardless of whether the mesh matches the shape or not, the overall convergence properties of FEM are not affected. There are three practical aspects of the implementation:

1. Space integration. We represent shapes as juxtapositions of arbitrary convex polyhedrons. We then compute a set theoretic intersection of these polyhedrons with FE mesh elements. This results in a set of pieces: convex polyhedrons resulting from volumetric intersections of the input polyhedrons and FE elements. For each element we create a list of pieces contained inside of it. Whenever volumetric integration needs to be done (e.g. to compute internal forces or stiffness/mass matrix) we integrate over these pieces, using the FE shape functions of the background mesh.

2. Boundary conditions. In our code [5] boundary conditions are prescribed by means of Lagrange multipliers. There is then no general difficulty with prescribing boundary conditions in this particular context. Contact detection and resulting contact constraints are based on the actual body shape. The resulting kinematic and dynamic derivations correspond to the background FE mesh, just as they would in the conventional sense.

3. Inertia properties. If a consistent mass matrix is used, the shape of the background mesh and the actual shape of a body do not need to be well aligned. When a lumped mass is used though, the background FE mesh should tightly approximate the actual shape. This is natural, since some of the information is lost in the process of lumping the mass properties. In our applications we use row-summed lumped mass and thus background meshes are usually tight.

7 EXAMPLES

The examples below are not aimed at demonstration of accurate predictions of small deformations of analysed bodies. Instead, we demonstrate that the dominant rigid motion can be well reproduced by means of the co-rotational formulation, while the deformability combined with the stiffness-proportional damping can be used to model post-impact
behavior. The practicality of such approach will yet need to be validated. Here, we only indicate its potential usefulness.

7.1 Free rotation of a body

In this example we rotate the body from Figure 1. Elastic material parameters are 1E10, 0.2, 2E3 for respectively the Young modulus, Poisson ratio and mass density. The initial angular velocity of value $2\pi$ is prescribed along the longitudinal direction. For this input the body makes one full rotation per one second of simulation.

We symmetrically pick two opposite points aligned with the $x$ direction at the internal cylindrical surface of the body (points $A$ and $B$ in Figure 1). The inner radius of the body is 0.1315 so that their initial distance $|A - B| = 0.263$. We picture this distance as function of time, which allows to show radial expansion of the body due to centrifugal effects. We also monitor the $y$ displacement of one of the picked points and compare it with a corresponding $y$ displacement of a rigid body model of the same problem. This way we can see whether the FE model is in phase with the gross rigid motion of the body.

The first goal of this example is to test how stable the co-rotational integration scheme is. Without damping, $\eta = 0$, and for a too large time step the extrapolated estimate of the half-step rotation in (10) will gradually diverge from the actual rotation of the body. This will cause excessive internal forces due to erroneous interpretation of deformational displacements in (12). Eventually this will lead to uncontrolled swelling of the body. In Figure 2 (left) an onset of this sort of behaviour can be observed in for time step 0.005, corresponding to 1.8 deg of incremental rotation per time step. Clearly, for too large time steps, undamped co-rotational scheme will produce poor results. The problem with stability can be fixed by including a small amount of stiffness-proportional damping, $\eta = 1E-3$. This is illustrated in Figure 2 (right), where the $y$ displacements of point $A$ are compared over 10 seconds of simulation for the FE and rigid bodies. The agreement between both models is very good.

In Figure 3 the time history of the inner diameter $|A - B|$ is plotted for the time step 0.001 and the damping parameter $\eta \in \{0, 1E-5, 1E-4\}$. The diameter stably oscillates for the undamped case. For damped runs the diameter comes to a steady state with its value dependent on the damping parameter. The larger the damping parameter, the larger the stabilized diameter. This corresponds to the fact that the outward radial component of the velocity contributes an artificial external force through the stiffness-proportional damping. Nevertheless, the amount of deformation due to this effect remains far below values of engineering interest.

Finally, Table 1 compares time integration runtimes for one second runs with time step 0.001, computed for rigid (6 degrees of freedom), co-rotational FE and Total Lagrangian FE models (288 degrees of freedom). The co-rotational formulation is about 16 times faster than the Total Lagrangian one. This ratio will increase for larger meshes.

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1Input file at: [http://code.google.com/p/soltec/source/browse/imp/body-rotate.py](http://code.google.com/p/soltec/source/browse/imp/body-rotate.py)
Figure 2: Body rotation, time step 0.005. Left: unstable, undamped run; time history of the inner diameter of the body. Right: stable, damped run ($\eta = 1E-3$); time history of the $y$ displacement of point A in Figure 1; FE and rigid motion histories overlap.

Figure 3: Body rotation, time step 0.001. Time history of $|A - B|$ for stable runs with and without damping, $\eta \in \{0, 1E-5, 1E-4\}$.

<table>
<thead>
<tr>
<th></th>
<th>rigid</th>
<th>CR-FE</th>
<th>TL-FE</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.14</td>
<td>8.56</td>
<td>137</td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Body rotation. Comparison of time integration runtimes for rigid, co-rotational FE and Total Lagrangian FE formulations. One second run with time step 0.001.
7.2 Flat impact of a body

In this example we vertically drop the body from Figure 1 onto a flat rigid obstacle. The material parameters are like in the previous example. We assume zero friction and use the velocity level Signorini impact model

\[ U_N \geq 0, \quad R_N \geq 0, \quad U_N R_N = 0 \]  

where \( U_N \) is the normal relative velocity between the body and the obstacle, and \( R_N \) is the normal impulsive force between the two objects. At the contact point level this corresponds to an ideally plastic impact: a point mass remains on the obstacle after hitting it. Similarly for a rigid body model this means that after hitting the obstacle the body will remain there, without rebound. If the body is deformable though, it will undergo a complex pattern of local and global deformations that will store and subsequently release some energy, resulting in a degree of rebound. This is a complex phenomenon, whose accurate modeling requires a fine discretization in order to capture inelastic effects near the impact zone and elastic stress waves that are excited and subsequently damped within the bulk of the body. This we cannot afford in a structure comprising thousands of bodies. The aim of this exercise is to see whether some post-impact behavior can be modelled given the relatively large space and time resolution that is available to us.

In this example the body is placed 1 meter above the flat rigid obstacle and it falls freely under gravity \((0,0,-10)\). When it hits the obstacle its vertical velocity is about \(-4.45 \text{ m/s}\). Due to the way the geometry is modeled, 20 contact points are created upon first impact, cf. Figure 4, and the inequality constraint (32) is implicitly enforced at all of them. The post-impact behavior of the body corresponds then to the interplay of the immediate loss of energy at contact points due to the ideally plastic character of the impact law (32), and to the dissipation of the energy in the bulk of the body due to the stiffness-proportional damping.

\[ ^2 \text{Input file at: http://code.google.com/p/solfec/source/browse/inp/body-impact.py} \]
The stable explicit time step for this example is about of 2E-5. Integrating in time with this step allows to account for all deformation modes and hence store a maximal possible amount of energy during impact. When using an implicit time integration we choose to skip some of the higher frequency modes in order to save computational time. As a consequence we operate on a subset of the modes and, with increasing step size, we gradually store less and less energy in deformations. This can bee seen in Figure 5 (left), where the post-impact behavior of undamped runs becomes increasingly more rigid for larger time steps. In the same figure on the right we can see the time history of the z displacement of point \( A \) for step 0.0005 and for a range of damping values. Clearly, we are able to reproduce post-impact behavior ranging from partially elastic to ideally plastic.

8 CONCLUSIONS

We have presented a computationally modest way of accounting for large rotations in the context of stiff deformable kinematics. Our time integration scheme, combined with the contact constraint (32) results in energetically consistent, dissipative scheme (also in case of friction). The degree of deformability and the time resolution can be freely adjusted depending on the available computer power or modelling needs, while the stiffness-proportional damping allows to independently obtain a range of post-impact behavior (without affecting the rigid motion). This seems particularly attractive in the context of multibody problems for which deformability of individual bodies contributes to a collective behavior. Of course, the greatest challenge and the matter of future work is to validate this approach on available experimental data. In the meantime, we would like to invite the readers to test our approach by downloading Solfec from http://code.google.com/p/solfec/.
ACKNOWLEDGEMENTS
The support from EDF Energy is gratefully acknowledged.

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A PORE-SCALE HYDRO-MECHANICAL COUPLED MODEL FOR GEOMATERIALS

E. CATALANO∗, B. CHAREYRE∗, A. CORTIS† AND E. BARTELEMY ††

∗Grenoble INP, UJF Grenoble I, CNRS UMR 5521, 3SR lab
BP53, 38041 Grenoble Cedex 9, France
e-mail: catalano@hmg.inpg.fr
web: www.3s-r.hmg.inpg.fr/3sr/

†Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, CA, 94806, U.S.A.

††Grenoble INP, UMR CNRS 5519, LEGI
BP 53, 38041 Grenoble Cedex 9, France

Key words: DEM, Fluid-solid coupling, Pore network, Consolidation

Abstract. We present a model for fluid-saturated granular media coupled flow and mechanical deformation. The fluid is assumed to be incompressible and the solid part is assumed to be a cohesive granular material. Forces exerted by the fluid in motion are determined and applied to solid particles. We derive a finite volumes formulation of the flow problem and we couple it to a discrete element method (DEM) formulation of the solid deformation.

The ability of the algorithm to solve transient problems is tested by simulating an oedometer test on a soil sample. The numerical solution of our model is in good agreement with Terzaghi’s analytical solution.

1 INTRODUCTION

Discrete element modelling is a tool to study the phenomena that take place at the scale of elementary components of materials. Such a technique is of great interest when applied to geomechanics problems. Modelling the hydro-mechanical coupled response of saturated porous media is indeed one of the main topics of rock and soil mechanics, and inspired one of the main contributions of Karl Von Terzaghi, whose theory of consolidation of soils “[...]has been one of the strongest incentives in the creation of a science of soil mechanics. (M.A.Biot)”. The model presented in this work aims at providing an effective tool for the analysis of the mutual influence between internal flow and deformation in geomaterials,
by modelling the interactions that take place at the particles scale. Depending on the type of problem, various strategies can be adopted for coupling the solid-fluid interaction, which differ essentially on how the fluid phase is being modelled.

At the microscopic (sub-pore) scale, the solid and fluid phases occupy different portion of the spatial domain and interact at their common interface. Thus, the microscopic fields which describe the properties of constituents may be considered as continua within a single phase, while exhibit discontinuities at the interfaces between phases. At such scale, fluid flow is governed by Stokes equations, which express fluid mass and moment conservation at small Reynolds and Stokes numbers

\[ \nabla p = \mu \nabla^2 u - \rho \nabla \Phi \]

\[ \nabla \cdot u = 0 \]

where \( u \) and \( p \) are the microscopic fluid velocity and piezometric pressure, respectively, \( \mu \) is the fluid dynamic viscosity, and \( \Phi \) is a potential field (e.g., gravitational field). The piezometric pressure \( p \) is related to the absolute pressure \( p^* \) via \( p = p^* - \rho \Phi \). A no-slip boundary condition for the fluid velocity at the grain boundaries is specified, \( u = 0 \), which is essentially responsible for the microscopic viscous energy losses (drag) that translate in a net loss of the macroscopic piezometric pressure, \( p \), over the length of a porous column. The numerical solution of Stokes equations in spheres assemblies is computationally expensive, especially for complex three-dimensional pore geometries. Finite Element Methods (FEMs) [13] or Lattice-Boltzmann (LB) [14] methods follow a microscopical approach but often find limitations (on the problem size, i.e.) linked to a heavy demand in terms of computer memory and computational cost.

The continuum approach is often adopted at the macroscopic level when modelling the fluid phase in order to get acceptable computational costs [8]. In such approach, there is no direct coupling at the local scale, and flow-induced forces on particles are defined as function of meso-scale averaged fluid velocity obtained from porosity-based estimations of the permeability. The use of phenomenological laws for the estimation of the permeability, however, limits severely the predictive power of these models, in conditions where parameter are poorly calibrated. Moreover the adoption of such approach does not allow the analysis of the individual particle behaviour, and so cannot be applied to problems whose nature is purely micromechanical, like strain localization or internal erosion.

The model we propose represents a middle way between the abovementioned approaches: the solid phase is characterized by a sphere packing DEM model, while the fluid phase moves through finite volumes in a pore network built upon a discretization of the spheres packing void space, referred hereafter as “Pore scale Finite Volumes’ (PFV).

Pore network models are based on a simplified representation of porous media as a network of pore and throats. They have been primarily developed to predict permeability of materials [11],[9] or in modelling multiphase flow effects from microstructure geometry [10], [15], [6], provided an appropriate interpretation on how fluids are exchanged between
pores and how such fluxes interact with the solid grains. These aspects will be developed and discussed in what follows. The ability of the model to reproduce the consolidation process will be finally tested.

2 THE GRAINS

The Discrete Element Method (DEM), as it is implemented in the open-source code YADE [19], was used to model the mechanics of the solid phase. The approach is fully micromechanical, the soil behaviour being modelled by defining the mechanical properties of the interaction between the grains [5]. Here, the soil grain’s shape is assumed to be spherical. This is a quiet usual assumption in DEM works, except in cases when the specific influence of the grain shape on the soil behaviour is under investigation. In other circumstances, use of polydisperse sphere packings is sufficient to reliably reproduce the soil behaviour [16].

At each DEM simulation time step, particles in contact are detected and then subjected to a repulsive force according to an elasto-plastic interaction law. The particles are then accelerated according to the second Newton’s law of motion, and their position is updated for the next step. A detailed description of YADE DEM implementation in YADE is available in the code’s documentation [20].

3 THE PORES

Delaunay triangulation and its dual Voronoi graph were used to discretize the void space and formulate the flow problem. Such geometrical representations are commonly used in soil mechanics for the definition of microscale stresses and strains [12] or in pore-scale modelling of single-phase or multi-phase flow [10]. The C++ library CGAL [17] is used for the triangulation procedure. Here, the generalization to weighted points of the Delaunay triangulation (Regular Delaunay triangulation) was adopted, where weights account for the radius of spheres [17]. A system of tetrahedra arises in a 3D framework, each one representing a pore (see fig.1(A) and fig.2). Such scheme constitutes a discretization of the void space in finite volumes, which will allow the approximation of the flow equations. The dual Voronoi diagram constitutes a network whose edges never cross non-void regions (see fig.1(B)) and form closed regions each one containing exactly one grain (coloured in fig.1(B)). Such network ideally represents the flow path of fluid within the porous sample and allows the formulation and resolution of the flow problem, as it will be detailed in the following.

4 FLUXES

The porous medium is assumed to be saturated with an incompressible fluid. For each tetrahedron of the triangulation, the volume of fluid coincides with the total volume \( \Theta_i \) (see fig.2) which is not occupied by any portion of the spheres. As a consequence, the continuity equation for pore \( i \), can be recast into a surface integral form using the
The continuity equation for pore $i$ each tetrahedron of the triangulation, the volume of fluid coincides with the total volume 4. FLUXES be detailed in the following. Porous sample and allows the formulation and resolution of the flow problem, as it will (coloured in fig.1(B)). Such network ideally represents the flow path of fluid within the equations. The dual Voronoi diagram constitutes a network whose edges never cross non-

tion of the void space in finite volumes, which will allow the approximation of the flow each one representing a pore (see fig.1(A) and fig.2). Such scheme constitutes a discretiza-

account for the radius of spheres [17]. A system of tetrahedra arises in a 3D framework, Regular Delaunay triangulation the Delaunay triangulation (coloured in fig.2A), and the fluid - solid interface, where $(u - v) \cdot n = 0$. The integration domain can therefore be restricted to $S_{ij}$ and the equation (3) rewritten in a discrete form as a sum of the fluxes that each pore exchanges with its neighbours.

$$V_i^f = \sum_{j=1}^{j_4} \int_{S_{ij}} (u_n - v_n) ds = \sum_{j=1}^{j_4} q_{ij} \quad (4)$$

4.1 Local Conductances

Our approach allows the definition of a local conductance $k_{ij}$ between adjacent pores $i$ and $j$ of an inter-pore gradient, defined as the ratio between the pressure drop $p_i - p_j$ and the length $l_{ij}$, the interpore distance. Based on the Voronoi diagram that was presented in previous sections, such length is assumed to be the euclidean distance between the Voronoi centres, labelled $P_i$ and $P_j$ in fig.2(D). The linear relation between the flux $q_{ij}$ and the local pressure gradient, can be expressed as follows:

$$q_{ij} = k_{ij} \frac{p_i - p_j}{l_{ij}} \quad (5)$$

Assuming the flow as laminar viscous and incompressible, Hagen-Poiseuille equation represents the ideal physical framework by which local conductances may be interpreted.
Considerable efforts have been devoted in the literature to the generalization of Poiseuille’s law to pores of complex shape [7], and to the definition of a generalized hydraulic radius [3]. By analogy with the Hagen-Poiseuille relation, \( k_{ij} \) may therefore be defined as follows:

\[
k_{ij} = \alpha \frac{S^f_{ij} R^h_{ij}^2}{\mu}
\]

where \( \alpha \) is a non-dimensional conductance factor which reflects the throat’s shape. For \( \alpha = 1/2 \), Hagen-Poiseuille equation takes the classical form which can be obtained for circular shaped conduits. \( \mu \) is the fluid dynamic viscosity. \( S^f_{ij} \) is the fluid domain of equation (4). The hydraulic radius \( R^h_{ij} \) is defined as the ratio between a volume filled with liquid and a wetted surface,

\[
R^h_{ij} = \frac{\text{Volume}_{\text{fluid}}}{\text{Surface}_{\text{wetted}}} = \frac{\Theta_{ij}}{\gamma_{ij}}
\]

for each pore connection, \( ij \). As already seen in previous sections, neighbouring pores have three grains in common, and thus three vertices of the triangulation resulting in a triangular plane facet. Those three vertices, together with the Voronoi centres (\( P_i, P_j \), see fig.2(D)) that are defined for the two pores, define a relevant pore partitioning and allow to access the total fluid volume \( \Theta_{ij} \) and the wetted surface \( \gamma_{ij} \), and the corresponding hydraulic radius (see fig.2(D)).

4.2 Forces

We will give very few details on the definition of forces exerted by the fluid to the solid particles. For a complete description on how the expressions that will be presented hereafter have been obtained, refer to Chareyre et al. [1].

The total force \( F^k \) on particle \( k \) can be defined as follows:
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\[
k_{ij} = \alpha S_{ij} R_{h ij}^2 \mu (6)
\]

where \( \alpha \) is a non-dimensional conductance factor which reflects the throat’s shape. For \( \alpha = 1/2 \), Hagen-Poiseuille equation takes the classical form which can be obtained for circular shaped conduits. \( \mu \) is the fluid dynamic viscosity. \( S_{ij} \) is the fluid domain of equation (4). The hydraulic radius \( R_{h ij} \) is defined as the ratio between a volume filled with liquid and a wetted surface,

\[
R_{h ij} = \frac{\text{Volume}}{\text{Surface}} = \frac{\Theta_{ij}}{\gamma_{ij}} (7)
\]

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\[4.2 \text{ Forces}\]

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The total force \( F_k \) on particle \( k \) can be defined as follows:

\[
F_k = \int_{\partial \Gamma_k} (p^* n + \tau n) ds \quad (8)
\]

where \( \partial \Gamma_k \) denotes the solid surface of the particle \( k \), \( p^* \) the absolute pressure and \( \tau \) the shear stress. As detailed in the introduction, the piezometric pressure \( p \) governing the flow problem is defined as \( p = p^* - \rho \Phi(x) \). By this definition, the \( F_k \) term can be splitted in three components:

\[
F_k = \int_{\partial \Gamma_k} \rho \Phi(x)n ds + \int_{\partial \Gamma_k} p n ds + \int_{\partial \Gamma_k} \tau n ds = F_{b,k} + F_{p,k} + F_{v,k} (9)
\]

where \( F_{b,k} \) denotes the buoyancy force, that can be computed independently, while \( F_{p,k} \) and \( F_{v,k} \) are those forces which result from viscous flow, respectively due to losses of piezometric pressure and to viscous shear stress.

\[5 \text{ PROBLEM SOLUTION}\]

The resolution of the flow problem can now be integrated into the algorithm presented in section 2. Combining equations (4) and (5), we obtain:

\[
\dot{V}_{f i} = \sum_{j=1}^{j_1} q_{ij} = k_{ij} \frac{p_i - p_j}{l_{ij}} = K_{ij} (p_i - p_j) \quad (10)
\]

At each cycle of computation, once the positions of the spheres are updated, new contacts are detected and the volumetric variation of pores is computed. The contact law and the fluid problem resolution give the contact forces and the fluid forces to be applied to particles, whose positions is again updated according to the law of motion (see fig.3). The matrix \( K_{ij} \) is sparse, symmetric and positive defined. The linear system is then solved by using an over-relaxed Gauss-Seidel algorithm.
6 PERMEABILITY MEASUREMENTS

The first tests that have been prepared to verify the relevance of the model implementation were based on the analysis of a flow through a fixed solid skeleton ($V_i^f = 0$ in eq. 10). A pressure gradient was then applied to the granular sample. The flow boundary conditions are the ones shown in fig. 5: pressure is imposed on top and bottom boundaries, while a no-flux condition is imposed on lateral boundaries. Thus, on top and bottom boundaries the pressure was imposed and fixed ($p = 1$ and $p = 0$ respectively). Inlet $Q_i$ and outlet $Q_o$ flow rates can be then measured. It was found that $Q_i - Q_o < 10^6 \approx 0$, which indicates a good convergence of the numerical solver. An estimation of a macroscopic Darcy-like permeability $[m^2]$ of the sample is then possible, being possible to assess the Darcy velocity of fluid flowing within the sample, $V_{Darcy} = Q/S$, with $S$ the section of the sample and $Q = Q_i = Q_o$. Permeability can be thus estimated from the following relation:

$$K = \mu \frac{Q}{S} \frac{h_0}{\Delta p} [m^2]$$

(11)

where $h_0$ is the height of the sample, $\Delta p$ the pressure drop and $\mu$ the viscosity of the fluid. Figure 4(a) compares the assessed permeability values with experimental data by Willie and Gregory [18], the Ergun equation and numerical results obtained by Thompson [11]. Figure 4(b) shows the pressure field associated to the given boundary conditions.

Table 1 shows a comparison between the PFV solution with the solution obtained by small scale Stokes flow FEM computations in terms of degrees of freedom to compute the pressure field and CPU time for solving. It can be seen how in the case of PFV calculation, the total number of DOFs and CPU time required for calculating flow and forces acting on the particles are reduced drastically with respect to small scale Stokes flow FEM calculations. Not available values are relative to computations whose occupancy of
memory was out the computer’s capacity. The pressure fields and effective permeabilities that were computed had been compared to FEM solutions and found in good agreement. For details, see Chareyre et al.\[1\].

Table 1: Comparison of DOF’s and CPU time between FEM and PFV (one iteration).

<table>
<thead>
<tr>
<th>Nb of spheres</th>
<th>FEM dof’s</th>
<th>PFV dof’s</th>
<th>FEM time [s]</th>
<th>PFV time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>1.7e5</td>
<td>45</td>
<td>300</td>
<td>0.00022</td>
</tr>
<tr>
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<td>1.2e6</td>
<td>1093</td>
<td>5400</td>
<td>0.0046</td>
</tr>
<tr>
<td>2e3</td>
<td>not available (n.a.)</td>
<td>12e3</td>
<td>n.a.</td>
<td>0.091</td>
</tr>
<tr>
<td>2e4</td>
<td>n.a.</td>
<td>11e4</td>
<td>n.a.</td>
<td>2.21</td>
</tr>
</tbody>
</table>

7 MONODIMENSIONAL CONSOLIDATION

The ability of the algorithm to solve transient problems was finally tested by analyzing the consolidation process of a sample subjected to axial load. Grains are free to move, so the system to be solved is the one expressed in eq.(10). Boundary conditions are set in order to reproduce an oedometer test, as it will be detailed hereafter. The analysis of the evolution of settlement and excess pore pressure in space and time and the comparison of the numerical solution with the analytical solution obtained by Terzaghi in 1923 in his “Theory of consolidation of soils” will constitute a validation for the model.

7.1 The Terzaghi’s analytical solution

The consolidation process is a classical hydro-mechanical problem. The mechanisms that govern the evolution of the deformation depend on a variation of effective stresses, coupled to processes of diffusion of the interstitial water. Such phenomenon depends therefore on the properties of the porous medium, like permeability and deformability, and on the problem geometry, defined by the boundary conditions and the drainage patterns which characterize the medium. The load applied to a saturated medium is initially entirely carried by the fluid phase, as the water can not instantly flow out of the medium. An increase of pore pressure is induced, whose entity varies within the medium, while the external pressure keep a constant value $u_0$. A gradient of pressure is then established, resulting in a filtration flux whose duration depend on the medium properties. As the water progressively flows out of the medium, the load is transferred from to liquid to the solid phase, and the medium starts to deform. The process ends once the excess pore water pressure is fully dissipated.

The equation of monodimensional consolidation reads:

$$\frac{\partial u}{\partial t} = C_v \frac{\partial^2 u}{\partial z^2}$$ (12)
where \( u \) is the fluid pressure, \( z \) the height of the sample, \( C_v \) the consolidation coefficient, defined as follows:

\[
C_v = \frac{K}{m_v g \rho_w}
\]

where \( K \) is the permeability of the soil expressed in \( \text{m/s} \), \( m_v = \Delta \varepsilon_v / \Delta \sigma'_v \) the coefficient of volume compressibility, \( g \) the gravity acceleration and \( \rho_w \) the density of the fluid. Terzaghi’s analytical solution is usually given in terms of consolidation degree \( U_z \), defined as the ratio between the excess pore pressure at instant \( t \) and the initial one, and average degree of consolidation \( U_m \), defined for a soil layer of height \( H \) as the ratio between the settlement \( S \) at the instant \( t \), \( (S(t) = \Delta H(t)) \), and the final settlement \( S_c \) (\( S_c = \Delta H_{\text{final}} \)).

\[
U_z = \frac{u(z,t)}{u_{\text{max}}} \quad (14)
\]

\[
U_m = \frac{S(t)}{S_c} \quad (15)
\]

A non-dimensional time parameter is introduced, \( T_v \), defined as:

\[
T_v = \frac{C_v t}{L^2} \quad (16)
\]

where \( t \) is the effective time, and \( L \) the longest drainage path of the generic fluid particle. \( T_v = 0 \) at the begin of consolidation, whereas \( T_v = 1 \) (100\%) at the end of the process.

### 7.2 Numerical results

Setting up the simulation, boundary conditions were defined according to the oedometric conditions, which mirror the main hypothesis of Terzaghi’s theory, briefly recalled hereafter: settlements and fluxes take place along one unique direction; the soil is homogenous and saturated; stress-strain relation is linear; the liquid and solid phase are incompressible; small and time-independent strains; validity of Darcy’s Law. Boundary conditions are shown in figure 5. Lateral strains are imposed to be none (\( \varepsilon_{xx} = \varepsilon_{yy} = 0 \)). A slip condition was set at the boundaries. Both upward and downward drainage ways were activated (\( L = H/2 \) in eq.16). A relative dense sample was created, to minimize the dispersion of pores’ dimension and avoid strong heterogeneities within the sample. 5000 slightly polydispersed grains were employed to build a cubic sample (\( l = 0.1m \)) which was then subjected to an axial external load \( \sigma_{\text{ext}} = 5kPa \). The external fluid pressure was set to be none, \( u_0 = 0 \).

The result that were obtained are shown in figure 6, with the evolution of excess pore pressure (left diagram) which rose up to \( 5kPa \) (\( = \sigma_{\text{ext}} = u_{\text{max}} \)) and then gradually decreased. A good agreement is found in terms of evolution of settlement and excess of pore pressure. The central diagram shows the evolution of \( U_z \), as defined in eq.14. The four curves are relative to four phases of the consolidation process, for \( T_v = 0.0 \) (0\%...
Four curves are relative to four phases of the consolidation process, for a non-dimensional time parameter is introduced, where \( t \). Material conditions are shown in Figure 5. Lateral strains are imposed to be none, with incompressible; small and time-independent strains; validity of Darcy’s Law. Boundary conditions are homogenous and saturated; stress-strain relation is linear; the liquid and solid phase are hereafter: settlements and fluxes take place along one unique direction; the soil is homogeneous.

### 7.2 Numerical results

Then subjected to an axial external load \( \sigma \), slightly polydispersed grains were employed to build a cubic sample. Dispersion of pores’ dimension and avoid strong heterogeneities within the sample. 5000 particles were activated. A slip condition was set at the boundaries. Both upward and downward drainage ways were activated. A relative dense sample was created, to minimize the relative error. Setting up the simulation, boundary conditions were defined according to the oedometric conditions, which mirror the main hypothesis of Terzaghi’s theory, briefly recalled hereafter: settlements and fluxes take place along one unique direction; the soil is homogeneous.

The result that were obtained are shown in Figure 6, with the evolution of excess pore pressure. The central diagram shows the evolution of settlement. A good agreement is found in terms of evolution of settlement and excess of pore pressure. (continued line) is compared to the numerical result (points) and found in good agreement.

### 8 CONCLUSIONS

We presented a pore-scale hydromechanical model for geomaterials that allows for a reliable and computationally efficient of the force exchange between fluid phase and solid particles, modeled a sphere packing. The pore-network model proved to be a relevant approach to interpret the physical phenomena that take place at the microscopic scale. The adoption of spherical grains assures an easy-to-handle pore geometry, and simplifies the derivation of local conductivities and fluid forces.

Comparison with small-scale Stokes flow FEM calculation shows how the CPU time required for solving the flow problem is drastically reduced by 6 orders of magnitude in our PFV-DEM approach. A good agreement has been found both in terms of pressure field and estimation of effective permeability. The ability of our approach to solve tran-
sient problems was tested by analyzing the consolidation process of a saturated sample
subjected to axial load. The solution obtained is in good agreement with Terzaghi’s
analytical solution (both in time and space).

The application of the model to problems concerning internal erosion [2] and sediment
transport in rivers are being tested. Current works focus on the reproduction of the
liquefaction phenomenon as it takes place within a seabed under the action of natural
ocean waves.

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GRAIN SCALE SIMULATION OF FLOW IN A SANDSTONE SAMPLE
BY USING THE MOVING PARTICLE SEMI-IMPLICIT (MPS) METHOD

LIANG-YEE CHENG*, RICARDO GOLGHETTO DOMINGOS* AND
MARCIO MICHIHARU TSUKAMOTO†

*Dept. Construction Engineering, Escola Politécnica
University of São Paulo
Av. Almeida Prado, Trav. 2 No. 83, Ed. Engenharia Civil, 05508-900 São Paulo, SP, Brazil
e-mail: cheng.yee@poli.usp.br, web page: http://www.pcc.usp.br

†Dept. Mining and Petroleum Engineering, Escola Politécnica
University of São Paulo
Av. Professor Melo Moraes, 2373, 05508-900 São Paulo, SP, Brazil
e-mail: golghetto@usp.br

Key words: Grain scale simulation, MPS.

Abstract. Since the grain scale modelling of flow in porous media is of great interest for the oil industry, the aim of the present research is to show an application of Moving Particle Semi-Implicit (MPS) method to the grain scale simulation of fluid flow in porous media. Geometry data obtained by a high-resolution CT scan of a reservoir sandstone sample was used as input for the simulations. The results of the simulations performed considering different resolutions are given, as well as the head loss and permeability obtained numerically.

1 INTRODUCTION

The grain scale modelling of flow in porous media is of great interest for the oil industry, since it allows the understanding of how the phase interfacial physics affect the fluid flow behaviour and macroscopic flow properties. Considering the development of new enhanced oil recovery methods, some studies on numerical approaches have been reported recently. Among the recent contributions, Holmes et al. [1] modelled the water-oil flow in porous media by using Smooth Particle Hydrodynamics (SPH). Despite the of the hypothetical porous media with relatively high porosity formed by spheres, the numerical results provide many insights about the relevance of surface tension on the effectiveness of the oil recovery. On the other hand, Ovaysi and Piris [2] carried out simulation based on Moving Particle
Semi-Implicit (MPS) method [3] and obtained the permeability of a sandstone sample.

The aim of the present research is to show an implementation for the grain scale simulation flow in porous media and the numerical results obtained from the simulations. For the three-dimensional modelling of the rock complex geometry and the flow inside its porous, MPS method developed for the simulation of incompressible flows was adopted. Numerical simulations were carried out employing data obtained by a high-resolution CT scan of a real reservoir sandstone sample. A pre-processing module was created to simplify the generation of the input data from the CT scan data. The results of the simulations performed considering different resolutions are also presented to investigate the impact of the microscopic scale modelling parameters on the macroscopic flow properties in order to achieve the compromising solution between accuracy and processing time.

2 MOVING PARTICLE SEMI-IMPLICIT (MPS) METHOD

The Moving Particle Semi-implicit (MPS) method adopted in the present study is a particle based fully lagrangian meshless method for incompressible flows. For the fluid domain, the governing equations are the continuity equation and the momentum conservation equation as follows:

$$\frac{D\rho}{Dt} = -\rho(\nabla \cdot \bar{u}) = 0 \quad (1)$$

$$\frac{D\bar{u}}{Dt} = -\frac{1}{\rho}\nabla P + \nu \nabla^2 \bar{u} + \bar{f} \quad (2)$$

where $\rho$ is the fluid density, $\bar{u}$ is the velocity vector, $P$ is the pressure, $\nu$ is the kinematic viscosity and $\bar{f}$ accounts for other accelerations.

All operators are represented by particle interaction models based on the weight function which depends on the particles relative positions:

$$w(r) = \begin{cases} \left(\frac{r_e}{r}\right)^2, & (r < r_e) \\ 0, & (r < r_e) \end{cases} \quad (3)$$

where $r$ is the distance between two particles and $r_e$ is the effective radius, which limits the region where interaction between particles occurs.

The gradient vector and the Laplacian operators are defined as functions of the relative positions between the particles. Whereas a scalar function $\phi$, the gradient vector and the Laplacian of a particle $i$, considering the neighboring particles $j$, are represented by Eqs. (4) and (5). The gradient vector used in this study is the formulation proposed by Tanaka and Masunaga [4].

$$\langle \nabla \phi \rangle_i = \frac{d}{pnd^0} \sum_{i \neq j} \left[ \frac{(\phi_j + \phi_i)}{|r_j - r_i|} (\bar{r}_j - \bar{r}_i) w\left(|\bar{r}_j - \bar{r}_i|\right) \right], \quad (4)$$

$$\langle \nabla^2 \phi \rangle_i = \frac{2d}{pnd^0\lambda} \sum_{i \neq j} (\phi_j - \phi_i) w\left(|\bar{r}_j - \bar{r}_i|\right) \quad (5)$$

where $d$ is the number of spatial dimensions, $r_i$ and $r_j$ are, respectively, the position vector of the particles $i$ and $j$, $\lambda$ is a parameter that represents the growth of variance and may be calculated using the Eq. (6).
The particle number density \( pnd \), calculated by Eq. (7), is proportional to the density and its initial value \( pnd^0 \) is used to ensure the condition of incompressibility of the flow.

\[
\lambda = \frac{\sum_{j \neq i} w(\|\vec{r}_j - \vec{r}_i\|) \cdot \|\vec{r}_j - \vec{r}_i\|^2}{\sum_{j \neq i} w(\|\vec{r}_j - \vec{r}_i\|)}.
\]

\[\text{(6)}\]

The MPS method is based on a semi-implicit algorithm where the pressure is calculated implicitly and all other terms such as gravity and viscosity are calculated explicitly. The Poisson’s equation can be deducted from the continuity equation and the pressure gradient:

\[
\langle \nabla^2 P \rangle_{i+\Delta t} = -\frac{\rho}{\Delta t^2} \frac{pnd^*_i - pnd^0}{pnd^0}
\]

\[\text{(7)}\]

Where, \( pnd^* \) is the particle number density explicitly calculated. The term of the left can be discretized using the Laplacian model, leading to a system of linear equations.

Particles are considered as free surface one when their \( pnd \) are smaller than \( (\beta \cdot pnd^0) \). According to Koshizuka and Oka [3], \( \beta \) may vary between 0.80 and 0.99.

Rigid walls are discretized as particles with no motion beneath the wall particles. Two layers of dummy particles are placed at the side that has no contact with the fluid to maintain the correct particle number density estimation.

As inflow boundary condition, fluid particles are injected to the domain by moving wall particles with their dummies at a constant velocity. When they displace a distance equal to the particle size, these wall particles are replaced by fluid particles. At the same time, the position of wall and their dummies are shifted back to their initial location restarting the loop.

For two-dimensional cases analyzed herein, \( r_e \) was set to 2.1l_0, where \( l_0 \) is the initial distance between particles, to calculate pressure gradient and the particle number density. \( r_e \) is 4.0l_0 for cases involving the Laplacian operator.

3 CASE OF STUDY

3.1 THE SANDSTONE SAMPLE

Numerical simulations have been carried out employing a real porous rock geometry, which has been obtained by a high-resolution CT scan of a reservoir sandstone sample whose porosity is 18.2%. The dimension of the sample is 1.0 x 1.0 x 1.0 mm. The CT scan generated data set of 300 x 300 x 300 points. In order to simplify the manipulation of the huge amount of the data, a pre-processing module has been created to simplify the conversion of the CT scan data to the input data for the numerical simulations. Fig. 1 shows a view of the complex networks of the porous inside the sandstone sample generated from the high-resolution CT scan data.
3.2 THE PRE-PROCESSING

The original CT scan data have identified only two regions: solid and void. To reduce the computational cost of the simulation, the resolution of the sandstone sample was reduced from 300 pts/mm to 50, 60 and 100 pts/mm. This was done by checking the most common particle type within cubes of 6, 5 and 3 points of side length, respectively. As the first step of pre-processing, points on void regions are converted into fluid particles. As the MPS method uses wall and dummies particles to model the solid surfaces, the pre-processor identify wall and dummy particles by setting a radius to check the status of a point and it neighbours. If all of the neighbour points inside the checking range are solids ones, it will be converted to a dummy particle; on the contrary it will be converted as a wall particle. Figure 2 shows a section view of the model in the 3 resolutions. The longitudinal section plan is set at 1/3 of the width of the sample because this is the position that provides good visualization of the flow inside the complex network of porous. Tab. 1 shows quantity of particles and absolute porosity of each model.
To ensure unidirectional flow, solid walls were added to the lateral faces of the models. Also, to simulate the inflow of fluid, transition regions of 0.20, 1.33 and 0.10 mm were added in the upstream sides of the simulation models of 50, 60 and 100 pts/mm, respectively, and inflow boundary condition is set on the top of the transitions regions.

The simulated fluid is water, with a density of $10^3$ kg/m$^3$ and a viscosity of $10^{-3}$ Pa.s, and it was injected with a velocity of 0.0125 m/s.

4 NUMERICAL RESULTS

4.1 PRESSURE LOSS

Simulations for the three resolutions were carried out with time step of $10^{-6}$ s and their results were used to calculate head loss and permeability. Figure 3 gives the snapshots of the flow and the pressure distribution for four different instant $t=0.0125, 0.0250, 0.0375$ and $0.0500$ s. The distribution of the injected fluid (cyan colour particles), gives good insight of how the flow advances through the complex network of pores. Also, for $t=0.05$ s, when the flow already achieved steady state, the fluid particles originally presented in the model (blue colour particles) entrapped on the left side of the section clearly show the blocking effects of the side walls used to assure unidirectional flow, and call for more carefully interpretation of the computed permeability. On the other hand, the sequence of the pressure distributions shows that quite stable computation was obtained in this case.

More detailed numerical results at $t=0.05$ s of the case with 100 pts/mm resolution is illustrated in Fig. 4, which provides three sections views of pressure distribution inside the
sandstone sample. The longitudinal section plans are located at 0.25 mm, 0.50 mm and 0.75 mm from the lateral face of the sample. These section views show that a smoothly varying pressure distribution was obtained in all the pores of the model.

Figure 5 shows the time series of the computed pressure at the entrance of the sample for the three cases. Instead of starting from zero pressure, as observed in the cases with 50 pts/mm and 100 pts/mm, a very high pressure was computed on the case with 60 pts/mm resolution. Perhaps it is caused by some unstable computation in the beginning of the simulation, but despite of the difference, the time series of all the three cases converge quickly to 2746 Pa, 2859 Pa and 1081 Pa for 50 pts/mm, 60 pts/mm and 100 pts/mm, respectively, with small oscillation around the mean values. Despite the pressure drop of the case with 60 pts/mm is slightly higher than the case of 50 pts/mm, the pressure drop decreases drastically for the case of 100 pts/mm showing the effect of the spatial resolution caused mainly by the blocking of particles in narrower pores.

Figure 3: Snapshots of the flow and pressure distribution obtained from the simulation of the model with 100 pts/mm resolution.
The pressure drop between the entrance and the exit of the sample was used to calculate the head loss and permeability of the sandstone. In this study, as the pressure at exit of the sample is set to zero, the pressure drop is equal to the pressure at the entrance of the block. A method for calculating pressure drop analytically is presented in the next section.

4.2 PERMEABILITY

The permeability can be determined by Darcy’s law and it is given by:
\[ k = \frac{Q \mu \cdot L}{\Delta P \cdot A} \]  

(9)

where \( k \) is the permeability, \( Q \) is the volumetric flow, \( \mu \) is the viscosity, \( L \) is the length of sample along flow direction, \( \Delta P \) is the pressure drop and \( A \) is the cross-sectional area of the sample.

Since flow is the product of velocity and area, this can be simplified into:

\[ k = \frac{V_s \mu \cdot L}{\Delta P} \]  

(10)

where \( V_s \) is the superficial velocity given by:

\[ V_s = \frac{Q}{A} \]  

(11)

where \( Q \) is the volumetric flow and \( A \) is the area of the cross-section of the sample.

Head Loss can be estimated by the Bernoulli’s equation. By neglecting the head loss due to the potential and kinetic components, we have:

\[ \Delta H = \frac{\Delta P}{\rho \cdot g} \]  

(12)

where \( g \) is the gravity acceleration.

From the computed pressure drops shown in the previous subsection, the computed values of head loss and permeability of the sandstone sample are given in Tab. 2.

<table>
<thead>
<tr>
<th>Resolution [pts/mm]</th>
<th>( \Delta p ) [Pa]</th>
<th>( \Delta H ) (m)</th>
<th>( k ) (mD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>2746</td>
<td>0.28</td>
<td>4612</td>
</tr>
<tr>
<td>60</td>
<td>2859</td>
<td>0.29</td>
<td>4430</td>
</tr>
<tr>
<td>100</td>
<td>1801</td>
<td>0.18</td>
<td>7032</td>
</tr>
</tbody>
</table>

4.3 VALIDATION

In order to check the magnitude of the results obtained by the numerical simulations, the pressure drop was estimated analytically by using Ergun equation:

\[ f_p = \frac{150}{Re_p} + 1.75 \]  

(13)

Where \( f_p \) is the friction factor and \( Re_p \) is the Reynolds number for porous media. Both are calculated as follow:

\[ f_p = \frac{\Delta P \cdot D_{GE} \cdot \varepsilon^3}{\rho \cdot V_s^2 \cdot (1 - \varepsilon) \cdot L} \]  

(14)

\[ Re_p = \frac{\rho \cdot V_s \cdot D_{GE}}{\mu \cdot (1 - \varepsilon)} \]  

(15)

where \( D_{GE} \) is the equivalent grain diameter, \( \varepsilon \) is the porosity of the sample.

Combining Eqs. (13), (14) and (15), we have:

\[ \Delta P = 150 \frac{\mu \cdot (1 - \varepsilon)^2 \cdot V_s \cdot L}{D_{GE}^2 \cdot \varepsilon^3} + 1.75 \frac{\rho \cdot V_s^2 \cdot (1 - \varepsilon) \cdot L}{D_{GE} \cdot \varepsilon^3} \]  

(16)

To estimate the equivalent grain diameter, it is assumed that they are spheres. Firstly, a
cross-section of the sample is chosen, and then its solid area is measured. Then, the number of grains inside the cross-section is obtained. Then, the average area of the grain is calculated, which will lead to the average diameter used as $D_{GE}$. Figure 6 illustrates the cross-section that was used to estimate the equivalent grain diameter of the sample used in this study.

![Figure 6: Cross-section used to estimate the equivalent grain diameter of the sample.](image)

The value of the pressure drop obtained analytical is 2035 Pa. For head loss it is 0.21 m and the analytically estimated permeability is 6143 mD. The results of the analytical estimation agree relatively well with the numerical results of the model with 100 pts/mm, which is the case with highest resolution simulated in the present study.

Moreover, the order of magnitude of permeability matches with those obtained by Ovausi and Piri [2], which used a sandstone sample of 22.2% porosity, and obtained permeability of 4250 mD for a sample of 1.02 mm x 1.02 mm x 1.02 mm (300 x 3000x 300 voxels), and 7380 mD for a 0.38 mm x 0.38 mm x 0.38 mm. According to [2], the values of permeability of the 22.2% porosity sandstone obtained by using Lattice-Boltzmann is 2220 mD and by using a reconstructed pore network is 3640 mD.

5 CONCLUDING REMARKS

In the present work, grain scale simulations of flow in porous media were carried out using CT scan data of a sample of reservoir sandstone which is modelled by Moving Particle Semi-Implicit (MPS) method. For the assessment of the pressure drop, head loss and permeability, there different spatial resolutions were considered.

The numerical results shows entrapping of some fluid particle, due to the rigid walls placed on the sides of the model to assure the unidirectional flow, might affect the calculation and might require the use of a larger representative elementary volume. Nevertheless, the values computed by the present study show relatively good agreement with the analytical estimation and are consistent when compared to the results available in the literature.

In this way, the numerical method used in the present study is effective for the study of grain scale media and, as suggested by Ovaysi and Piti [2], more detailed studies are necessary to verify the convergence of the numerical results, as well as the validation through the experimental measurements.
ACKNOWLEDGMENTS

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REFERENCES

INVESTIGATION OF INTERNAL EROSION PROCESSES USING A COUPLED DEM-FLUID METHOD

H. SARI*, B. CHAREYRE *, E. CATALANO*, P. PHILIPPE† AND E. VINCENS ‡

*Grenoble-INP , UJF-Grenoble 1, CNRS UMR 5521, 3SR
Grenoble F-38041, France
e-mail: bruno.chareyre@grenoble-inp.fr

† Cemagref – Geomechanics Group – OHAX.
Aix-en-Provence F-13182 , France

‡ Université de Lyon, LTDS Ecole Centrale de Lyon UMR CNRS 5513
Ecully F-69134, France

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Abstract. The evolution of granular beds subjected to upward seepage flow is investigated using a coupled DEM-fluid model implemented by Catalano et al. in the open-source software Yade-DEM. Firstly, filtration properties of a coarse narrowly graded material are analyzed by simulating the transport of smaller particles from a base layer through the coarse filter by gravitational loading or downward flow with uniform pressure gradient. The results are analysed on the basis of the constriction size distribution (CSD) of the filter which describes statistically the sizes of throats between pores in the material. Secondly, we examine the results obtained when, instead of two different layers, the coarse and fine materials are initially mixed in one unique layer and subjected to gravity. Thirdly, this mixture of coarse and fine particles is subjected to both gravity and a non-uniform pressure gradient, by injecting the fluid in one point below the layer, as inspired by previous experiments. Similar channeling patterns are obtained in both experiments and simulations when the boundary condition at the injection point is an imposed flux. This boundary condition results in a recirculation mechanism that remains confined in a finite zone around the injection point as long as the flux is below a threshold value. By simulating an imposed pressure condition, we finally show that instabilities can be triggered by the transport of small particles away from the injection point. This segregation process results in a lower porosity and an increased pressure gradient above the eroded zone, so that the instability-triggering pressure gradient in bi-dispersed mixtures is lower than in mono-dispersed mixtures.

1 INTRODUCTION

The stability of granular soils subjected to seepage flow is a major concern in civil engineering, particularly for the safety of hydraulic structure like dike or dams. The difficulty to carry out experiments in the laboratory can be overcome thanks to the capability of DEM
simulations to model the process of transport of fine particles through a coarse granular material. In this paper, a DEM-fluid model, previously developed by Catalano et al. [1][2] in the open-source software Yade-DEM [3], is used to analyze the migration of fines particles in different configurations of granular beds (i.e. coarse and fine base particles either in two separate layers or mixed in a unique layer) and with various fluid flow conditions.

2 DEM-PFV COUPLING MODEL

The numerical model is based on the coupling between a discrete element model (DEM) for the solid particles and a flow model for the interstitial fluid. Particles are represented as spheres, and the interaction between particles are of the elastic-plastic type, with normal and tangential stiffness $k_n$ and $k_s$, and Coulomb friction angle $\phi$. Particles motion is governed by Newton's laws of acceleration and more details of the algorithms can be found in [4].

The fluid flow model is based on a pore-scale discretization of Stokes equations for incompressible fluids, where pores are defined by tetrahedra resulting from the regular Delaunay tesselation of the sphere packings. Although similar ideas have been proposed by previous authors [15,16], the derivation and implementation of a 3D formulation for deformable spheres packings have only been done recently [2].

The governing equations are averaged at the pore scale. The emerging formulation is of the finite volumes type, referred below as PFV (« Pore scale Finite Volumes »). At each time step, the geometry and rate of deformation of each pore is updated on the basis of particles motion. In turn, the fluxes are determined and fluid forces on particles are computed and integrated in the laws of motion for each particle. The only parameter of the flow problem is the viscosity of the fluid $\eta$, taken equal to that of pure water in what follows.

DEM-PFV coupling is well suited for studying particles transport induced by seepage flow, as opposed to the more common coupling methods where the resolution of the flow discretization is above the particles scale (DEM-CFD coupling, see e.g. [5]). Indeed, DEM-PFV models define forces on particles that are not collinear with the macroscale pressure but, instead, reflect the local voids geometry and connectivity. On the other hand DEM-CFD couplings can only define average fluid forces on groups of particles, and the direction of forces is imposed by the mean fluid velocity at the macroscale. The definition of the fluid forces in the DEM-PFV model has been validated in [1].

3 FILTRATION TEST WITH TWO LAYERS

3.1 Dry filtration under gravity

The filter, composed of 4000 spherical particles, is created thanks to a sphere growth process which produces a homogeneous sample with a uniform porosity [12]. The filter is generated with a friction angle equal to 10° between the coarse particles and the corresponding porosity is 0.35. The same value is kept in all the simulations. In the filter, all the particles are blocked and its thickness is about $25\times D_{50}$ in the vertical direction and its width is $22\times D_{50}$ in the two horizontal directions. In most of simulations, narrowly graded materials are used with a ratio between the maximal and the minimal diameter equal to 3 and 2 for the coarse and fine particles respectively. These ratios are similar to the ones used in previous suffusion experiments by Sail et al. [6] which are considered a benchmark for this
work. The fines particles (4000) initially at rest above the coarse layer, are dropped under gravity on the filter (fig.1). No particles are dropped near the lateral walls ($2 \times D_{\text{max}}$) since at this distance the arrangement of particles within the filter is disturbed due to wall effects.

![Figure 1: Filter of spherical particles and fine particles on the top surface.](image)

Most of the literature about filter criteria as the well-known work by Sherard et al. [7] proposes to use the ratio $D_{15}/d_{85}$, which is called the Terzaghi criterion, recommended by ICOLD\(^1\) for the design of filters. Following this approach, the filtration properties will be analyzed as a function of this ratio. The friction between the coarse and the fine particles is another important parameter and four different friction angles will be tested.

Fig.2 gives the percentage of the successful passing particles through the filter. One can note that increasing the local friction between the fine and coarse particles, there are more trapped spheres. This result was also found by Reboul (2008) [8] who considered a local friction equal to 0 for a conservative study of DEM filtration in granular materials. As the local friction angle increases, the fine particles lose kinematic energy more quickly. As a consequence, their ability to pass through a constriction and to continue their movement is more rapidly restricted. The distribution of trapped particles within the filter is compatible with an exponential distribution as can be seen in Fig. 3(a) where the different layers are numbered from the top to the bottom of the filter. Note that such exponential distributions are recovered in experiments, as the ones that have been carried out in Cemagref (Aix-en-Provence, France) for the TRANSOL\(^2\) project thanks to an index-matching technique. A typical result is presented in Fig.3(b).

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\(^1\) International Commission of Large Dams
\(^2\) Transport of mass through granular soil (2007-2010). National project financially supported by the French Agency of Research (ANR)
Fig. 2: Passing particles according to $D_{15}/d_{85}$ ratio and the friction between the fine and coarse particles.

Fig. 3: Vertical distribution of trapped particles in the filter; (a): DEM-PFV simulation, (b): experiment on glass beads, after [13].

Fig. 4 shows the Constriction Size Distribution (CSD) of the filter and the Particle Size Distribution (PSD) of the base particles in different cases of filtration. The CSD criterion is used for the filtration properties because it is more precise than the Terzaghi criterion and better reflects the physical phenomena involved in filtration tests (Silveira (1965) [9], Witt (1993) [10], among others). Actually, the CSD reflects the geometrical retention capacity of a material since constrictions correspond to the narrowest paths between pores. For the computation of the CSD, a control volume excluding the filter particle which arrangement could be influenced by wall effects has been defined. We can see for example that for the fine’s PSD giving 99% of passing, nearly all the base particles are smaller than the smallest constriction, say the constriction made with the three smallest filter particles in mutual contact. One can also notice that the smaller constrictions which are more numerous in the medium are mainly responsible for trapping particles since only 20% of constrictions are responsible for trapping 50% of particles. For the 1% PSD, the smallest fine particle diameter is greater than the mode of the distribution which gives the value of the largest occurrence of
constriction size in the medium. Since the probability of having pores connected by constriction sizes greater than this mode is low, the probability of a successful transit across the filter decreases dramatically [8].

![Figure 4: Particle Size Distribution (PSD) of fine particles associated to different passing percentage.](image)

### Table 1: Filter efficiency according to the ratio $D_{15}/d_{85}$.

<table>
<thead>
<tr>
<th>Material</th>
<th>Cu</th>
<th>$D_{15}/d_{85}$</th>
<th>Filter</th>
<th>Indraratna et al [11]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base particles</td>
<td>1.29</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coarse filter</td>
<td>1.47</td>
<td>15.4</td>
<td>50 % passing</td>
<td>Ineffective</td>
</tr>
<tr>
<td>Medium filter</td>
<td>1.49</td>
<td>5.2</td>
<td>1 % passing</td>
<td>Effective</td>
</tr>
</tbody>
</table>

Other simulations were performed with other values of coefficient of uniformity Cu of the filter, i.e. other $D_{\text{max}}/D_{\text{min}}$. These are values chosen by Indraratna et al [11] (table 1). The thickness of their filter is nearly $200\times D_{50}$ whereas, the one involved in this study is $25\times D_{50}$. So, if we take into account this and the fact that the distribution is exponential, a filter which get through 50% of the particles with a thickness of $25\times D_{50}$ must be ineffective, as found by Indraratna with a thickness of $200\times D_{50}$. For 1 % of the particles passing by the filter, since the probability of further movement through the filter decreases with the filter thickness, it will be even more effective for a $200\times D_{50}$ filter thickness.

### 3.2 Downward flow

In this section, the same kind of simulations is performed but gravity is removed and replaced by a downward hydraulic flow. To limit computational time, a smaller thickness of $8\times D_{50}$ is used for the filter. The hydraulic flow is induced by imposing a pressure gradient of 150 Pa/m. This new situation is analyzed for two $D_{15}/d_{85}$ ratios equal to 3 and 1.5. The
friction angle during the creation of the sample and between fine and coarse particles is 10°.

Table 2: Percentage of passing particles for dry filtration and involving a water flow.

<table>
<thead>
<tr>
<th>( D_{15}/d_{85} )</th>
<th>Gravity</th>
<th>Flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>66 %</td>
<td>84 %</td>
</tr>
<tr>
<td>1,5</td>
<td>1,3 %</td>
<td>5 %</td>
</tr>
</tbody>
</table>

Table 2 shows that the flow allows passing more numerous particles than with the gravity alone. This result is quite logical and it can be explained by the fact that we have a unique vertical force with the gravity whereas due to the tortuosity of the coarse particles filter, the flow also generates forces in the horizontal axes and allows the reorientation of the paths towards lateral constriction in pores. Figure 5 gives a more detailed view of the results given in Table 2.

Fig. 5(a) and 5(b) show the distributions of trapped particles either with the flow or with gravity and for the two \( D_{15}/d_{85} \) ratios. These distributions are obviously very different depending on the size ratio. At a given ratio, there is an almost systematic but very low decrease of trapped particles in each horizontal layer and the form of the dropped particle distribution is nearly the same between gravity and flow.

For \( D_{15}/d_{85}=1,5 \), as expected, most of particles are trapped within the first layer. The larger particles block some paths but, since they are not that numerous, other large enough paths are still available for the penetration of finer particles within the sample. This simulation reflects the phenomenon of superficial filter clogging. For \( D_{15}/d_{85}=3 \), the filtration of fine particles takes place more gradually and seems to be more related to the maximum probable path length a particle of a given diameter can flow through a granular filter.

![Figure 5](image_url)  
Figure 5: Trapped particles after filtration by gravity or by downward flow for (a) \( D_{15}/d_{85}=3 \) and (b) \( D_{15}/d_{85}=1,5 \).
4 FILTER AND FINE PARTICLES MIXED IN ONE LAYER

In this section, we present the results obtained when coarse and fine particles are initially mixed in one unique layer. In the first part we briefly present results obtained with gravitational loading alone, to verify that there is a potential movement of fine particles in such configuration. However, the primary objective here is to investigate the migration of particles in materials subjected simultaneously to both gravitational loading and fluid forces, when the flux is oriented upward (opposed to gravity). We simulate a point injection at the bottom of the box, as inspired by experiments carried out at the Cemagref by Philippe [13-14].

4.1 Simulations with gravity

We present the results obtained with $D_{15}/d_{85} = 4$, for different proportions of fine and coarse particles. All particles are free to move, with the exception of coarse particles inside the bottom layer, which have the degrees of freedom blocked along the z-axis, as if they were supported by a coarse sieve. The thickness is about $8 \times d_{50}$ in the three directions.

In table 3, we examine how many fine particles will fall out of the packing as function of the initial fine/coarse distribution. Note that 0% passing is never expected in this configuration, since fines from the bottom boundary will always fall freely (they don't have to cross the filter). The relevant information is the number of fines blocked inside the filter in the final configuration. Note also that when the initial number of fines is high, a settlement of the whole packing is expected while fines are moving down progressively, emptying the gaps between big particles. The results show that $D_{15}/d_{85} = 4$ in a mixed packing allows potential movement of at least a fraction of the small particles.

<table>
<thead>
<tr>
<th>% of fines by weight</th>
<th>0,5%</th>
<th>5%</th>
<th>10%</th>
<th>20%</th>
<th>30%</th>
<th>40%</th>
</tr>
</thead>
<tbody>
<tr>
<td>% of successful passing</td>
<td>49,00%</td>
<td>47,00%</td>
<td>53,00%</td>
<td>48%</td>
<td>77,00%</td>
<td>99,00%</td>
</tr>
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</table>

4.2 Local upward fluid injection

Finally, we present the simulations including gravity and an upward fluid flow. The boundary condition defining the influx is an imposed pressure in the first step, and an imposed flux in the second step. The $D_{15}/d_{85}$ ratio is 3, the percentage of fines is 30 % and all particles are free to move. These values have been chosen to highlight the suffusion process. The sample thickness is about $6 \times d_{50}$ and the width about $17 \times d_{50}$ in the horizontal directions.

Suffusion of the fine particles is generally obtained in the simulations as soon as the influx is high enough, both with imposed pressure or imposed flux (Fig.6). Similar effects have been observed in experiments, [e.g 6].
With an imposed pressure, we observe a threshold value (near 10kPa) beneath which the system is stable and the flow is constant. For a pressure higher than this value, and after enough simulation time, a small cavity appears around the injection point. As soon as this erosion process is initiated, the flux increases rapidly (Fig. 8), and the cavity grows larger. This process generally results in a large cylinder-shaped void crossing the packing vertically, together with a recirculation mechanism of fine particles. These effects are qualitatively
similar to what was reported by Philippe [13,14] – see fig. 7. The difference is that the particles size distribution is uniform in Philippe’s work and that is why the suffusion zone is larger in our case, due to the coarse particles. Some of the particles are also moved out of the layer and stay suspended until they fall down and touch the packing again, like in a suspension.

**Figure 8:** Flux versus time (number of iterations) for an imposed pressure of 10kPa at the injection point.

**Figure 9:** Flux and pressure values with an imposed flux value of 2 m$^3$/s.
With an imposed flux, there is also a minimal value of the flux in order to trigger some movements of particles. For an imposed flux higher than this limit value, some of the small grains migrate away from the injection point (it is noticeable that, unlike fine particles, the coarse part of the filter is stable for the range of fluxes we present here).

The major difference between imposed pressure and imposed flux lies in what happens after the initiation of erosion processes. Fig. 9 shows the values of both the flux and pressure for an imposed flux of 2 m$^3$/s. We shall note that the value of the flux cannot be imposed directly. Instead, it is needed to adjust the value of the pressure via a servo-control algorithm in order to maintain the flux to a prescribed value. One can notice in fig. 9 that the control does not prevent fluctuations around the prescribed value. This is due to the strong coupling between fluid flow and particles re-arrangements which, in turn, modify the conductivity of the packing. Nevertheless, the average flux is close to 2 m$^3$/s whereas the pressure decreases rapidly while the erosion mechanisms tend to increase the conductivity of the system. As a result, there is no rapid evolution of the system as in the previous case (i.e. imposed pressure). The layer is always compact. The cavity near the injection point reaches a constant size, and no particles are ejected above the packing.

**CONCLUSION**

Numerical simulations of elementary tests involving filtration and erosion processes have been presented. The preliminary results are generally in agreement with experimental results. Although more investigations are needed to further validate the coupled model, we believe that DEM is relevant for understanding the fundamental mechanisms governing the complex phenomena of particles migration and instabilities in granular materials. In this context the DEM-PFV coupling has the advantage of reflecting mechanisms occurring at the particles scale (movement of fines, but also the effect of local heterogeneities of the solid fraction) with acceptable computation times and memory footprint.

Current work aims at simulating more realistic configurations, like the ones tested in Philippe [13], with larger numbers of particles. Still, the number of simulated particles will not approach the number of particles in most of the experiments. It will raise interesting questions on similarity conditions and scaling laws in internal erosion problems in order to compare simulations and experiments.
REFERENCES


KELVIN-HELMHOLTZ INSTABILITY BY SPH

M. S. Shadloo∗, M. Yildiz†

Faculty of Engineering and Natural Sciences, Advanced Composites & Polymer Processing Laboratory, Sabanci University, 34956 Tuzla, Istanbul, Turkey.
∗e-mail: mostafa@sabanciuniv.edu, www.msshadloo.com
†e-mail: meyildiz@sabanciuniv.edu

Key words: Smoothed Particle Hydrodynamics (SPH), Shear flow, Two-Phase flow, Interfacial flows, Surface tension, Kelvin-Helmholtz Instability (KHI).

Abstract. In this paper, we have modeled the Kelvin-Helmholtz Instability (KHI) problem of an incompressible two-phase immiscible fluid in a stratified inviscid shear flow with interfacial tension using Smoothed Particle Hydrodynamics (SPH) method. The time dependent evolution of the two-fluid interface over a wide range of Richardson number (Ri) and for three different density ratios is numerically investigated. The simulation results are compared with analytical solutions in the linear regime. It was observed that the SPH method requires a Richardson number lower than unity (i.e., Ri \approx 0.8) for the onset of KHI, and that the artificial viscosity plays a significant role in obtaining physically correct simulation results that are in agreement with analytical solutions. The numerical algorithm presented in this work can easily handle a two-phase fluid flow with various density ratios.

1 INTRODUCTION

Flow instability at the interface between two horizontal parallel streams of different velocities and densities, with the heavier fluid at the bottom, is called the Kelvin-Helmholtz Instability (KHI). The KHI is induced by either velocity shear within a continuous fluid or a sufficiently large velocity difference across the interface of a multiphase fluid. The instability kicks in when the destabilizing effect of shear across the interface overcomes the stabilizing effect of stratification due to gravity and/or surface tension if it exists. The KHI manifests itself as a row of horizontal eddies (in the form of waves) aligned across the interface. These eddies or waves are referred to as main billows. There are several well-known natural situations where the KHI can be observed such as wind blowing over the ocean or water surface, a meteor entering the Earth’s atmosphere, the interface between the tails of comets and solar wind, or the interface between a liquid layer and a compressible gas, among others.
The Kelvin-Helmholtz instability problem was solved first for the ideal case of inviscid and incompressible fluids in 1871 by Lord Kelvin. It has been studied both theoretically [1] and experimentally [2], as well as numerically [3, 4].

Smoothed Particles Hydrodynamics (SPH) is one of the most successful Lagrangian methods which was introduced separately by Gingold and Monaghan and Lucy in 1977 initially to simulate astrophysical problems. Due to its flexibility and capability of modeling complex engineering problems, the SPH method has been extensively used for solving a wide variety of problems [5, 6]. As well, there are some recently reported works which have been conducted to investigate the feasibility and the ability of the SPH method to capture the physics behind the KHI [7, 8].

The aim of this work is to simulate the KHI by using a Weakly Compressible SPH (WCSPH) method, thereby showing the ability of the SPH technique to capture this hydrodynamic instability for various density ratios. The current presentation differs from earlier works in the following aspects: the previously reported relevant works treated the fluid to be compressible whereas here it is treated as an incompressible liquid. Unlike other pertinent SPH papers, this paper systematically examines the effects of the stabilizing parameters (e.g., surface tension (\(\sigma\)) and stratifying body force (\(\Delta\rho g\))) individually or concurrently on the occurrence of the KHI for a wide range of \(Ri\) numbers and three density ratios.

2 SMOOTHED PARTICLE HYDRODYNAMICS

SPH is a Lagrangian particle-based method which has been extensively used over a decade for solving partial differential equations (thermo mechanical balance laws integrated with relevant constitutive equations) for both fluids and solids dynamic problems. In comparison to mesh-dependent approaches, the SPH method significantly facilitates the handling of the problems with free or interfacial surface, whose locations are priori unknown and have to be computed during the solution of the problem since the position of particles determine the final configuration of the flow domain. Therefore, it is a particularly powerful tool to study multiphase fluid flow problems.

The term \textit{particles} merely refers to movable points that represent fluid elements in three dimensional space, and each particle is associated with mass, density, velocity and other relevant hydrodynamics properties. In another way of saying, the continuum under the consideration is discretized into finite number of field points which are known as particles. Field variables carried by each particle are calculated through an interpolation (weighting, smoothing, kernel) function, \(W(r_{ij}, h)\) from those of surrounding neighbor particles. Here, \(r_{ij}\) is the magnitude of the distance vector \((\vec{r}_{ij} = \vec{r}_i - \vec{r}_j)\) between the particle of interest \(i\) (an interpolated particle) and its neighboring particles \(j\) (neighbors of the interpolated particle), and \(h\) is called smoothing length, which is an important input parameter that controls the number of active neighbor particles within the support domain of smoothing function. Here, \(\vec{r}_i\) and \(\vec{r}_j\) are the position vectors for particles \(i\) and \(j\), respectively. The weighting function should have the following attributes; the normalization, the Dirac-delta
function, the compactness, and spherically symmetric even function properties. Due to the compactness property, \( W(r_{ij}, h) = 0 \) when \( r_{ij} > h \), in computations, a given particle interacts with only its nearest neighbors contained within the radius of support domain \( h \).

For an arbitrary function (scalar \( A \), vectorial \( \vec{A} \), or tensorial \( A \)), the kernel approximation in the form of the integral representation can be written as

\[
A(\vec{r}_i) \triangleq \langle A(\vec{r}_i) \rangle = \int_{\text{Space}} A(\vec{r}_j)W(r_{ij}, h)d^3\vec{r}_j. \tag{1}
\]

where the angle bracket \( \langle \rangle \) denotes the kernel approximation.

In the SPH method, it is common practice to replace the integral operation with a summation over all the particles within the support domain of the kernel function (i.e. \( r_{ij} < h \)). In what follows, one can write

\[
A_i = A(\vec{r}_i) = \frac{1}{\psi_i} \sum_j A_j W_{ij} \tag{2}
\]

where we have used a concise notation (i.e. \( W(r_{ij}, h) = W_{ij} \)), and the differential volume element \( d^3\vec{r}_j \) is approximated by the reciprocal of the number density \( \psi_i \), which is defined for the particle \( i \) as

\[
\psi_i = \sum_j W_{ij}, \tag{3}
\]

By using a differentiable kernel, the spatial derivative of the function \( A \) evaluated at the location of particle \( i \) can be simply reduced to an ordinary differentiation of the interpolant function \( W_{ij} \) with respect to the particle \( i \) times the volume and the field variables of neighbor particles. It is due to this analytical approximation that the SPH method does not require a grid. For example, one of the widely used SPH gradient discretization scheme of the field \( A \) can be written in the form of

\[
\nabla_i A_i = \nabla_{\vec{r}_i} A(\vec{r}_i) = \frac{1}{\psi_i} \sum_j (A_j - A_i) \nabla_i W_{ij}. \tag{4}
\]

where \( \nabla_{\vec{r}_i} A(\vec{r}_i) \) or in a concise notation \( \nabla_i A_i \) denotes the spatial derivative of the field \( A \) with respect to \( i^{th} \) particle coordinates. Since the kernel function determines the extent of the interaction between the particle of interest and its neighbors, its choice is related to the accuracy, efficiency, and stability of the resulting algorithm. In this work, the quintic kernel based on the fifth-order spline function is adopted [9].
2.1 Governing Equations

The governing equations used to solve the fluid problems in this article are the mass and linear momentum balance equations which are expressed in the Lagrangian form and given in the direct notation as

\[
\frac{d\rho}{dt} = -\rho \nabla \cdot \vec{v},
\]

\[
\rho \frac{d\vec{v}}{dt} = -\nabla p + \rho \vec{g} + \vec{F}^\sigma,
\]

where \( p \) is the pressure, \( \vec{v} \) is the fluid velocity, and \( \vec{F}^\sigma \) denotes a force per unit volume exerted on the fluid-fluid interface due to surface tension. Here, it should be pointed out that in reality, the surface tension force on the fluid-fluid interface is a surface force (i.e., force per unit area). For the sake of computational efficiency and simplifications, we here have followed a common practice whereby the surface tension force per unit area is included in the momentum balance equation as the force per unit volume. As written in eq.(12), this volume force is proportional to product of the interface gradient (gradient of the color field used to distinguish two fluids) and the surface curvature. This approach is referred to as the continuum surface force (CSF) formulation and is widely used in modeling surface tension force of multiphase fluid flows. Also, it should be noted that due to the inviscid fluid assumption, the linear momentum balance equation does not have a viscous force term.

In the WCSPH method, for enforcing the incompressibility condition, the density can be evolved either using eq. (5) in combination with eq. (4) or directly utilizing the number density approach as given in eq. (7).

\[
\rho_i = m_i \psi_i
\]

As for the balance of linear momentum equation, the acceleration term can be discretized in the general form of

\[
\vec{a}_i = \frac{1}{m_i} \vec{F}_i,
\]

where \( \vec{F}_i \) is the total force acting on the particle \( i \), which can be written in the discrete form as

\[
\vec{F}_i = m_i \vec{g} + \vec{F}^\sigma_i - \sum_j \left[ \left( \frac{p_i}{\psi_i^2} + \frac{p_j}{\psi_j^2} \right) + \Pi_{ij} \right] \nabla_i W_{ij}.
\]

Here, the first term in the summation sign \( (p_i/\psi_i^2 + p_j/\psi_j^2) \) is the discretized form of the pressure gradient force and \( \Pi_{ij} \) is artificial viscosity.
The artificial viscosity term is included in the current model in order for circumventing numerical instabilities due to the meshless nature of the SPH method. This term introduces some numerical diffusion into the model, thus preventing non-physical oscillations. There are various forms of artificial viscosity terms in SPH literature. In this work, we have implemented the one suggested by Monaghan in [10] in the form of

$$\Pi_{ij} = -\frac{8\mu_{ij}(\bar{v}_{ij} \cdot \bar{r}_{ij})}{\psi_i \psi_j (r_{ij}^2 + \epsilon h_m^2)}$$  \hspace{1cm} (10)

where $\bar{v}_{ij} = \bar{v}_i - \bar{v}_j$, $\bar{r}_{ij} = \bar{r}_i - \bar{r}_j$, $h_m = \frac{h_i + h_j}{2}$, $\epsilon \approx 0.0001$ is introduced to prevent singularity when $r_{ij} = 0$ and $\mu_{ij}$ is harmonic average of $\mu_i$ and $\mu_j$ defined by

$$\mu_{ij} = \frac{2}{\frac{1}{\mu_i} + \frac{1}{\mu_j}}$$  \hspace{1cm} (11)

where $\mu_i = \frac{1}{8}\alpha h_i c_i$ in which $c$ is sound speed and $\alpha$ is the artificial viscosity constant.

In accordance with the continuum surface force (CSF) formulation, the surface tension force term in eq.(9) is formulated as

$$\bar{F}_i^\sigma = \sigma_i \kappa_i \bar{n}_i \delta_s,$$  \hspace{1cm} (12)

where $\kappa_i$ is the interface curvature, and $\bar{n}_i$ is the unit vector normal to interface and $\delta_s$ is the interface dirac delta function ($\delta_s = |\nabla C|$).

The unit vector normal to the fluid-fluid interface $\bar{n}_i$ is

$$\bar{n}_i = \frac{\nabla_i C_i}{|\nabla_i C_i|}.$$  \hspace{1cm} (13)

where $\nabla_i C_i$ is computed as.

$$\nabla_i C_i = \sum_j C_{ji} \frac{\bar{v}_{ij}}{\psi_{ij}} \nabla_i W_{ij}.$$  \hspace{1cm} (14)

where $\bar{v}_{ij} = (\psi_i + \psi_j)/2$ and $C_{ji} = C_j - C_i$.

Finally, the interface curvature $\kappa_i$ is calculated from

$$\kappa_i = \sum_j \frac{1}{\psi_{ij}} \bar{n}_{ij} \cdot \nabla_i W_{ij},$$  \hspace{1cm} (15)

where $\bar{n}_{ij} = \bar{n}_i - \bar{n}_j$. 
2.2 Time Integration

In order to increment the time-steps in the SPH algorithm, we have used a Velocity Verlet predictor corrector method [10]. This technique is an explicit time integration scheme, and is relatively simple to implement. The time integration scheme starts with the predictor step to compute the intermediate particle positions based on current particles’ velocities as follow

\[ \dot{\mathbf{r}}_i^{n+\frac{1}{2}} = \mathbf{v}_i^n + \frac{\Delta t}{2} \mathbf{a}_i^n. \]  

(16)

where \( n \) is the temporal index.

Afterward, new densities for each particles are calculated from eq.(3) and eq.(7) at current intermediate particle positions. Since fluid is assumed weakly compressible, the artificial equation of state of the form

\[ p - p_o = c^2 (\rho - \rho_o), \]  

(17)

is used to compute new pressure values at current particle positions. This state equation enforces the incompressibility condition on the flow such that a small variation in density produces a relatively large change in pressure hence preventing the dilatation of the fluid. Here, \( c \) is artificial sound velocity and the subscript \( o \) denotes the reference condition. The speed of sound for each particle must be chosen carefully to ensure that the fluid is very closely incompressible. In this work, upon selecting the sound speed twenty times larger than the maximum fluid velocity, the density variation is limited to one percent. Having computed the acceleration of each particle from eq.(8) using the current pressure and velocity values, one can obtain the velocity of new time-step through the time integration as

\[ \mathbf{v}_i^{n+1} = \mathbf{v}_i^n + \frac{\Delta t}{2} \mathbf{a}_i^{n+\frac{1}{2}} \]  

(18)

Finally, the position of each particle is corrected at the new time-step based on this velocity. It is to be noted that in the SPH method, the order of particles affects the accuracy of interpolations for gradient and Laplacian computations. Therefore, for the computational stability and accuracy, it is preferable to move the SPH particles in a more orderly fashion, which can be achieved through using the XSPH technique proposed by Monaghan et.al [10]. The XSPH method includes the contribution from neighboring particles, thereby causing a fluid particle to move with an average velocity

\[ \dot{\mathbf{r}}_i^{n+\frac{1}{2}} = \dot{\mathbf{r}}_i^{n+\frac{1}{2}} + \frac{\Delta t}{2} \bar{\mathbf{v}}_i^{n+1}. \]  

(19)

where \( \bar{\mathbf{v}}_i^{n+1} \) is the XSPH-averaged new velocity by the correction factor of 0.1.
3 Definition of The Problem

The KHI can occur at the interface between two horizontal parallel streams of different velocities and densities, with the heavier fluid at the bottom. For the simulation of this natural flow phenomenon, we here consider two immiscible fluids that are intervened between two infinite parallel horizontal plate with the height of $H$ ($0 < y < H$) (Fig.1). For simplicity, the $x$-dimension of the computational domain $L$ ($0 < x < L$) is chosen to be equal to the domain height $H$ ($L = H$).

The computational domain for the KHI problem is represented by a set of particles created on a Cartesian grid with an equidistant particle spacing. At the beginning of the simulations, the computational domain is halved by a horizontal midline ($H_1 = H_2 = \frac{H}{2}$ and $H = 1m$), where each half represents a different fluid region. The number of particles for each fluid region is the same. An initial sinusoidal perturbation is applied to the fluid-fluid interface through switching the type of particles near the midline. The wavelength of the initial disturbance is set to be equal to the domain length ($\lambda = L$) so that the instability is to be confined into mid section of the model domain. The magnitude of the perturbation is $\zeta_0/H \approx 0.03$ where $\zeta_0$ is the initial amplitude of the applied disturbance.

Let $U_1$ and $\rho_1$ be the velocity and density of the basic state of the upper layer and $U_2$ and $\rho_2$ be those of the bottom layer. Particles of two fluids initially at rest are set into motion in opposite directions with the same magnitude (i.e. $U_1 = -U_2 = U = 0.5\pi$).

To be able to show the effect of density on the KH instability, in simulations we have used several density ratios $\frac{\rho_2}{\rho_1} = 2, 5$ and $10$ where $\rho_1$ is set to be $\rho_1 = 1000 \frac{kg}{m^3}$. When all modeling parameters are active, the surface tension force acts ($\sigma$) only on the interface particles in the direction of the unit normal whereas gravity ($g$) acts in the downward direction on all particles. For determining the number of SPH particles for the particle number independent results, we run several test cases where three different particle arrays, namely, $80 \times 80$, $150 \times 150$ and $300 \times 300$ were used. It was observed that the $150 \times 150$ array of particles is sufficient for capturing primary wave as well as obtaining particle-
independent solutions.

4 RESULTS

For unstable situations, the analytical non-dimensional growth rate $G_e$ in the linear regime can be written as [11]

$$G_e = \text{Im}(\omega) = \frac{2\pi \sqrt{\rho_1 \rho_2}}{\rho_1 + \rho_2} \sqrt{1 - Ri}. \quad (20)$$

where $Ri$ is the dimensionless Richardson number

$$Ri = \frac{\rho_1 + \rho_2}{k \rho_1 \rho_2 (U_1 - U_2)^2} \left( g (\rho_2 - \rho_1) + k^2 \sigma \right). \quad (21)$$

For numerical investigation, the numerical growth rate $G_n$ is calculated in the form of

$$G_n = \frac{\hat{\zeta}/\zeta_o - 1}{t^*}, \quad (22)$$

where $\hat{\zeta}$ is the amplitude of the disturbance at time $t$ and $t^*$ is the dimensionless time.

$$t^* = \frac{t |U_2 - U_1|}{H}, \quad (23)$$

where $t$ is real time and $H$ is domain height.

To be able to compare the analytical growth rate in eq.(20) with the numerical one in eq.(22), (because eq.(20) is only valid for the linear regime), $\hat{\zeta}$ and $t^*$ are calculated when the wave amplitude reaches to 10 percentage of the domain height ($\hat{\zeta} \cong 0.1H$).

Having perturbed the fluid-fluid interface at the initial time ($t^* = 0$) by a small disturbance, under certain input parameters (i.e., surface tension, gravity, density, etc.), the interface disturbance grows and the flow system becomes unstable. Fig.2 illustrates the growth of the interface disturbance as a function of time in the two-dimensional KHI problem for the density ratios of $\rho_2/\rho_1 = 2$ and $\rho_2/\rho_1 = 10$ at $Ri = 0.01$. For this simulation, the artificial viscosity coefficient in eq.(10) is set to be $\alpha = 0.001$. As a result of the interface disturbance, the heavier fluid starts moving in a positive vertical direction, while the lighter fluid in the opposite direction. Thus, both fluids begin to penetrate into each other. As the time progresses, the height of the instability gets larger, and due to the inertial effect, both fluids tend to gain horizontal velocity opposite to their initial bulk velocities. A small vortex appears and the flow regime is no longer linear. This process results in the formation of the main billow. It should be noted that the linear stability growth rate formula is valid only before this time step. At later times, the characteristic form of the KHI becomes much more obvious. Passing time, the non-linear flow regime results in the formation of a Cat’s Eye vortex and the fingering phenomenon for the density ratios of $\rho_2/\rho_1 = 2$ and $\rho_2/\rho_1 = 10$, respectively.
Figure 2: Time evolution of the interface in the two-dimensional KHI problem with the density ratios of $\frac{\rho_2}{\rho_1} = 2$ and $\frac{\rho_2}{\rho_1} = 10$, and the $Ri = 0.01$; (a) $t^* = 1.0$, (b) $t^* = 2.0$, (c) $t^* = 3.0$, (d) $t^* = 4.0$; (I) particle distributions and (II) velocity vectors.
In the simulation with the density ratio of 2, both fluids have relatively close inertial forces, and therefore, the vortex is not advected significantly by fluid streams. Consequently, as the simulation progresses, the flow circulation forms the Cat’s Eye shape. On the other hand, due to the fact that there exists a relatively large difference in the inertial forces between the upper and the lower fluid layers for the density ratio of 10, and the heavier fluid at the bottom of the modeling domain has a greater inertial force than the lighter fluid at the top, the flow circulation is advected faster in the flow direction of the heavier fluid whereby it leaves the flow domain through the left side and re-enters it from the right side. Accordingly, the translational motion of the flow circulation along the interface brings about the elongation of the crest of the wave, or the fingering phenomenon.

From eq. (20) it is also notable that for a given density ratio, the $Ri$ number is the only parameter that controls the stability of the two fluid system in the KHI phenomena. Towards this end, it is important to determine the critical value for this number, which defines the border between stable and unstable flow regimes. The results of the simulations have shown that in the SPH method, the critical value for the $Ri$ number is approximately 0.8 for all density ratios, which is slightly smaller than the one determined using the linear stability analysis. This difference might be attributed to the artificial viscosity utilized in the SPH method, numerical diffusion and the methodology used to perturb the initial fluid-fluid interface.

Fig. 3a shows a plot of the growth rate versus the $Ri$ number in which numerically and analytically computed growth rates are compared. One can see from the figure that the numerically computed growth rate decreases with increasing $Ri$ number and/or density ratio, which is consistent with eq. (20), and simulation results are in close agreement with those corresponding to analytical solutions. The comparison of results presented in figs. 2 and 3 for the density ratios of 2 and 10 for a given $Ri$ number reveals that the density ratio significantly affects the shape of the main billow as well as the growth rate. It is also important to note that with increasing density ratio, the transition from a linear to non-linear regime is delayed to later simulation times.

The artificial viscosity is one of the reasons that may cause numerically obtained simulation results to deviate slightly from analytical ones. Fig. 3b illustrates the effect of the artificial viscosity on the time evolution of the interface in the two-dimensional KHI problem for one specific test case, which is chosen as a representative for the whole data. In this specific test case, $\rho_2/\rho_1 = 10$. As seen from the figure, upon choosing a low artificial viscosity coefficient, the numerical results are in better agreement with those of the linear stability analysis. One can also notice that the growth rate decreases as the utilized artificial viscosity coefficient increases. To have stable numerical simulations, the artificial viscosity coefficient can not be chosen to be too small (as an example, $\alpha \geq 0.0001$ and 0.001 for $\rho_2/\rho_1 = 2$ and for $\rho_2/\rho_1 = 10$, respectively). Therefore, it should be selected carefully in order to have physically valid numerical results, which can predict the KHI phenomena accurately without losing numerical stability.
Figure 3: Growth rates $G$ of KHI in the linear regime for various Richardson numbers and (a) the effect of density ratios ($\alpha = 0.001$) and (b) the effect of artificial viscosities ($\rho_2/\rho_1 = 10$).

5 CONCLUSIONS

The SPH method has been used to simulate Kelvin-Helmholtz instabilities in two-dimensional incompressible two-phase flows under the inviscid assumption through taking the effect of surface tension and body forces into account. Simulations were performed for numerous Richardson numbers, density ratios and artificial viscosities. It was shown that under the influence of certain input parameters (body force, surface tension, and density ratios), a flow instability develops in a two-phase fluid system with an initially disturbed fluid-fluid interface. This instability grows in time and, subsequently, the flow system experiences a transition from a linear to a non-linear regime. It was also illustrated that all simulations results are in reasonably good agreement in terms of growth rate with those corresponding to analytical solutions of the linear stability analysis for KHI. The noted discrepancies between numerical analytical results might be attributed to numerical diffusions, to the inclusion of artificial viscosity and to the nature of the initial disturbance of the fluid-fluid interface. Additionally, it was observed that the growth rate is higher for lower density ratio and Richardson numbers, and reaches to free shear flow limit at Richardson numbers near zero. Based on the linear stability analysis, for Richardson numbers lower than unity ($Ri < 1$), the flow can be unstable, but for the numerical method used in this paper, the flow instability occurs at ($Ri$) number values less than roughly 0.8. Numerical results suggest that for a given density ratio, the growth rate of the instability is only controlled by the Richardson number, and independent of the nature of stabilizing forces. Also it is shown that the artificial viscosity plays a significant role in all simulation, therefore, it should be chosen such that it preserves the stability of the numerical method as well as captures all complex physics behind this phenomenon.
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NUMERICAL INVESTIGATION OF THREE-PHASE FLOWS USING INCOMPRESSIBLE SMOOTHED PARTICLE HYDRODYNAMICS

Amir Zainali†, Nima Tofighi† and Mehmet Yildiz†

†Faculty of Engineering and Natural Sciences, Advanced Composites and Polymer Processing Laboratory, Sabanci University, Orhanli 34956, Tuzla, Istanbul, Turkey
e-mail: meyildiz@sabanciuniv.edu, http://people.sabanciuniv.edu/meyildiz/

Key words: SPH, multiphase flows, meshfree, phase specific surface tension

Abstract. An ISPH method for the simulation of three-phase flows is presented in this article. The proposed method is investigated through the simulation of a droplet located at the interface of two immiscible fluids as well as diamond droplet deformation. The extendibility of the proposed surface tension formulations for three-phase flows to two-phase flows is also investigated. It is observed that the results obtained from the numerical simulations are in good agreement with the analytical ones.

1 Introduction

Two-phase flows are investigated extensively numerically in the literature during the past decades while the physics behind the three and more phase flow problems are relatively unknown despite the fact that Multi-phase flows play an important role in many industrial and physical phenomena. Typical examples with many applications in chemical and biomedical industries include mixture of three or more fluids (e.g. oil-water-gas mixture in oil industry) and compound droplets. The main reason for the scarcity of numerical simulations for three-phase flows in comparison to two-phase flows can be due to the complications associated with the modeling of hydrodynamical interactions at the interface for three-component systems [3, 4, 6].

In this work, we have developed a 2-D multiphase incompressible smoothed particle hydrodynamics (ISPH) model based on the standard projection method initially used by Cummins and Rudman [2] for SPH, while the continuum surface force model proposed by Brackbill et al. [1] is used to model surface tension forces. The method proposed by Smith et al. [6] is implemented to take into account different surface tension coefficients between the phases in a three-component system.
This paper is organized as follows. In section 2, the mathematical formulations as well as numerical scheme are briefly described. In section 3, numerical results are presented. Finally in section 4 concluding remarks are provided.

2 Governing Equations

All constituents of the multiphase system are considered to be viscous, Newtonian and incompressible liquids with constant material properties, \( \partial \Gamma / \partial t = 0 \), where \( \partial / \partial t = \partial / \partial t + (v_k) \) is the material time derivative operator. The set of equations governing the motion of the flow under consideration are conservation of mass and linear momentum. In their local form for volume and discontinuity surface, these equations may be specified as

\[
\begin{align*}
D \rho / Dt &= - \rho v_k, \quad \text{on V-}\sigma \quad (1) \\
\rho D v_l / Dt &= \tau_{kl,k} - \rho b_l, \quad \text{on V-}\sigma \quad (2) \\
\|\rho (v_k - u_k)\| \hat{n}_k &= 0, \quad \text{on } \sigma \quad (3) \\
\|\rho v_l (v_k - u_k) - \tau_{kl}\| \hat{n}_k &= f^\sigma, \quad \text{on } \sigma \quad (4)
\end{align*}
\]

where V-\( \sigma \) denotes total volume, excluding the points lying on the surface of discontinuity, \( \sigma \). Equations (1) and (2) are valid within the body excluding \( \sigma \) while equations (3) and (4) are valid only on the surface of discontinuity and represent the jump condition across \( \sigma \). \( \tau_{kl} = -p \delta_{kl} + 2 \mu d_{kl} \) is the symmetric total stress tensor, \( d_{kl} = 0.5 (v_{kl} + v_{lk}) \) is the symmetric deformation tensor, \( \delta_{kl} \) is the Kronecker delta, \( p \) is the thermodynamic pressure, \( b_l \) is the body force, \( f^\sigma \) is the surface force per unit area on the interface due to surface tension for the mixture, \( v_k \) is the divergence-free velocity, \( \rho \) and \( \mu \) are the density and viscosity of the mixture. The symbol \( \|\phi\| \) indicates the jump of the enclosed quantity across the discontinuity surface, \( \phi^+ - \phi^- \) where \( \phi^+ \) and \( \phi^- \) are the values of \( \phi \) on the positive and the negative sides of the discontinuity surface. Here, \( u_k \) denotes the velocity of the discontinuity surface, \( \hat{n}_k \) is the unit normal to the discontinuity surface.

One can write the local form of the jump condition for the momentum balance as

\[
f^\sigma = \|p\| n_l = \gamma \kappa \hat{n}_l \quad (5)
\]

where surface tension coefficient, \( \gamma \), is assumed to be constant. Here, \( \kappa = -n_{m,m} \) is the curvature. For the sake of computational efficiency and simplification, it is preferable to express local surface force as an equivalent volumetric force (the force per unit volume). This can be achieved by using the continuum surface force model (CSF) proposed in [1]. Using this approach equation (5) can be expressed as a volume force by multiplying the local surface tension force with a one-dimensional delta function defined on the interface, \( \delta \),

\[
f^{\sigma \nu} = \sigma \kappa \hat{n}_l \delta \quad (6)
\]
In this study, to track the interface each particle is assigned to a color function,

\[ C^\alpha_i = \begin{cases} 
1, & \text{if } i \text{ belongs to fluid } \alpha \\
0, & \text{else} 
\end{cases} \tag{7} \]

and finally, 1-D delta function on the interface is chosen to be \( \delta = |C_m| \).

In the treatment of multiphase immiscible fluids with two constituents, the implementation of the continuum surface force model is straightforward in that there is only one interface between the constituents. On the other hand, in the multiphase systems with more than two constituents, an interface fluid particle may see two or more interfaces at the same time and in what follows a decision should be made as to which surface tension coefficient is to be used. To be able resolve this difficulty, in [6] the surface tension coefficient was decomposed into phase specific surface tension such that

\[ \gamma_{\alpha\beta} = \gamma_\alpha + \gamma_\beta \]

where \( \gamma_{\alpha\beta} \) is the physical surface tension coefficient between the phase \( \alpha \) and the phase \( \beta \), and \( \gamma_\alpha \) and \( \gamma_\beta \) are the phase specific surface tension coefficients for \( \alpha \)th and \( \beta \)th phases respectively.

For three-phase system,

\[
\begin{align*}
\gamma_{12} &= \gamma_1 + \gamma_2, \\
\gamma_{13} &= \gamma_1 + \gamma_3, \\
\gamma_{23} &= \gamma_2 + \gamma_3.
\end{align*}
\]

Upon solving a linear system of equations for \( \gamma_1, \gamma_2 \) and \( \gamma_3 \), one can write the following relations among the physical and phase specific surface tension coefficients

\[
\begin{align*}
\gamma_1 &= 0.5 (\gamma_{12} + \gamma_{13} - \gamma_{23}), \\
\gamma_2 &= 0.5 (\gamma_{12} - \gamma_{13} + \gamma_{23}), \\
\gamma_3 &= 0.5 (-\gamma_{12} + \gamma_{13} + \gamma_{23}).
\end{align*}
\]

As such, for each particle, three phase specific normals, curvatures, and the surface tension forces are computed. The total surface tension force acting on the given interface particle is then the sum of three phase specific surface tension forces such that

\[ f_{\sigma v}^i = \sum_{\alpha=1}^{3} f_{\sigma v}^{(\alpha) i} \]

where the subscript \( i \) is a particle identifier, and the adjacent Latin letter is the \( l \)th component of the surface force.

### 2.1 SPH preliminaries and the numerical method

The numerical method used in this work for linearizing the governing equations and associated interface and boundary conditions is based on the Incompressible Smoothed Particle Hydrodynamics method presented in [5], which is briefly described in what follows.

SPH particles interact with each other by means of an interpolation (weighting, smoothing, kernel) function \( W(r_{ij}, h) \), concisely designated as \( W_{ij} \) for a constant \( h \). Here, \( r_{ij} \) is the magnitude of the distance vector \( \vec{r}_{ij} = \vec{r}_i - \vec{r}_j \) between the particle of interest \( i \) and its neighboring particles \( j \), and \( h \) is referred to as the smoothing length which controls the interaction length among particles.

In the SPH method, an arbitrary function (i.e, scalar \( f(\vec{r}_i) \), vectorial \( f^p(\vec{r}_i) \), or tensorial \( f^{ps}(\vec{r}_i) \)) may be approximated as

\[ f_i^p = \int_{\Omega} f^p W_{ij} d^3\vec{r}_j \] where \( f^p(\vec{r}_i) \) is briefly denoted by \( f_i^p \).

Upon replacing the integral operation with a summation sign over all the particles within the cut-off distance (i.e. \( r_{ij} < Kh \), where \( K \) is a constant coefficient for the selected kernel function), and approximating the infinitesimal volume element by reciprocal of the number density \( \psi_j \), defined for the particle \( j \), one can write the SPH approximation of \( f_i^p \).
as

\[ f_p^i = f_p^i (r_i) = \sum_j \frac{1}{\psi_j} f_j^p W_{ij} \]  

(8)

where the number density for particle \( i \) is defined as \( \psi_i = \sum_j W_{ij} \).

Upon using a differentiable smoothing function, the spatial first order derivative of the function \( f_p^i \) evaluated at the location of particle \( i \) can simply be approximated through multiplying the gradient of the kernel function \( \partial W_{ij} / \partial x_i^s \) (taken with respect to the particle \( i \)) by the field variables and volumes of neighbor particles. There are several ways to discretize the first order spatial derivative of a field variable. Throughout this work, the one used is of the following form

\[ \frac{\partial f_p^i}{\partial x_i^k} a^k_{ij} = \sum_j \frac{1}{\psi_j} (f_j^p - f_i^p) \frac{\partial W_{ij}}{\partial x_i^s} \]  

(9)

where \( a_{ij}^{ks} \) is a corrective second-rank tensor given by,

\[ a_{ij}^{ks} = \sum_j \frac{r_{ij}^k}{\psi_j} \frac{\partial W_{ij}}{\partial x_i^s} \]  

(10)

This form is referred to as the corrective SPH gradient formulation that can be used to eliminate particle inconsistencies. It should be noted that the corrective term \( a_{ij}^{ks} \) is ideally equal to Kronecker delta, \( \delta^{ks} \) for a continuous function. As for SPH approximation to
the second order derivative of a vector-valued function, it can be written in two different ways as

\[ \frac{\partial^2 f_p}{\partial x^i \partial x^k} \partial_{ij}^{pm} = 8 \sum_j \left( f_p^i - f_p^j \right) \frac{r_{ij}^p}{r_{ij}^2} \partial W_{ij} \partial x^m, \]  

(11)

\[ \frac{\partial^2 f_p}{\partial x^i \partial x^k} \left( 2 + a_{ik}^{ss} \right) = 8 \sum_j \left( f_p^i - f_p^j \right) \frac{r_{ij}^p}{r_{ij}^2} \partial W_{ij} \partial x^i. \]  

(12)

For the time integration in the ISPH approach, two-stage predictor-corrector method with a first-order Euler time step scheme is used. The algorithm starts with the predictor step where the intermediate positions \( \vec{r}_i^* \) for all particles are calculated through the knowledge of preceding particle positions \( \vec{r}_i^{(n)} \) and the previous correct velocity field \( \vec{v}_i^{(n)} \) as

\[ \vec{r}_i^* = \vec{r}_i^{(n)} + \vec{v}_i^{(n)} \Delta t. \]

The intermediate velocity field \( \vec{v}_i^* \) is calculated on the intermediate particle locations by solving the momentum balance equations with forward time integration without the pressure gradient term as \( \vec{v}_i^* = \vec{v}_i^{(n)} + \vec{f}_i^{(n)} \Delta t \). The pressure Poisson equation is solved to obtain the pressure, \( p_i^{(n+1)} \), which is required to enforce the incompressibility condition. The actual velocity field at time step \( (n+1) \), \( \vec{v}_i^{(n+1)} \), can be obtained by using the computed pressure. Finally, with the correct velocity field for time-step \( (n+1) \), all fluid particles are moved to their new positions

\[ \vec{r}_i^{(n+1)} = \vec{r}_i^{(n)} + 0.5 \left( \vec{v}_i^{(n)} + \vec{v}_i^{(n+1)} \right) \Delta t. \]

3 Results and Discussion

In this section, results of the conducted simulations are presented. Computational domain for every simulation is taken to be a square with the side length of 1. Each row and column consists of 100 equally spaced particles for test cases evolving from a Cartesian particle arrangement. Test cases with non-Cartesian particle arrangement have the same number of particles as with their Cartesian counterparts. All fluid properties are set to unity for every phase involved in simulations while binary surface tension coefficient assumes a value of 0 or 1, depending on the test cases considered. Different phases are ordered as shown in figure 1. No-slip boundary conditions for the top and bottom, and side walls are applied. Zero pressure boundary condition is applied for all boundaries.

In order to test the applicability of the three-phase surface tension treatment to two-phase flow systems, the deformation of the initially diamond-shaped droplet under the effect of the surface tension force is considered. Particles of fluid 3 are initially positioned on a diamond surrounded by fluid 1 and 2 particles. The binary surface tension coefficient between fluids 1 and 2 is set to zero so as to make them act like a single fluid. Figure 2 provides the sequences of shape-evolution of the diamond bubble in the aforementioned test case in detail. The initial diamond evolves in time hence becoming a circle as the simulation continues. The circle obtained in this way is also used for the initial positioning of particles in some other test cases. As expected, the new surface tension treatment method presented for SPH of three-phase fluid flow is also applicable to a two-phase fluid
Figure 2: The time evolution of a diamond shaped bubble to a circle shape bubble; Left: particle positions, Right: color contour showing bubble boundary.
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In this study, two different methods are used for the initial arrangement of particles in a circular bubble positioned in a rectangular domain for the liquid lens. In the first method, all the particles are placed on a Cartesian grid and the bubble is formed through assigning different phases to each particle in accordance with their positions. The circular bubble obtained by this method is rather crude thereby presenting many irregularities in shape which eventually result in an intermittent surface tension force as shown in figure 3-a. In the second method, an initial diamond shaped bubble is allowed to deform into a circular bubble in a two phase flow as described previously. The simulation using an initial circular bubble generated by the second method leads to improvements in the surface tension force and particle positions, as seen in figure 3-b. The initial diameter for the crude bubble used here is 0.293 while the bubble obtained from the diamond shape has a diameter of 0.299. The reason behind this difference is that it is almost impossible to create a circular bubble shape of desired initial diameter (in this work, the initial diameter of interest is 0.3) from limited number of equally spaced particles on a Cartesian grid. The crude circle experiences an abrupt change in particle positions at early stages of the simulation due to the aforementioned irregular surface tension force. This affects the initial reading for the diameter, rendering it difficult to compare the results with analytical data. This problem is more evident in figure 4-a, where lens diameter versus time is shown for both test cases. While both test cases show the same characteristics, the crude bubble has smaller elongation rate along the major axis. The results are more evident when the transverse diameter of the lens is normalized by the analytically obtained equilibrium diameter, as shown in 4-b.
Figure 4: Change in transverse lens diameter versus time for different initial conditions; Solid line: crude circle marked in Cartesian distribution, Dashed line: circle obtained from evolution of a diamond.

Figure 5: The time evolution of the liquid lens visualized by color contours.

The shape of the droplet is controlled by the values of the surface tension forces. Therefore, under the effect of these surface tension forces, the initially circular droplet deforms into an elliptic or lens shape. The equilibrium three-phase contact angle is formulated as \( \sin \phi_1/\gamma_{23} = \sin \phi_2/\gamma_{13} = \sin \phi_3/\gamma_{12} \). The transverse diameter of the lens along the major axis (the distance between triple junctions) is computed through [4]

\[
d = \left( \frac{2(\pi - \varphi_1) - \sin(2\pi - 2\varphi_1)}{8A \sin^2(\pi - \varphi_1)} + \frac{2(\pi - \varphi_3) - \sin(2\pi - 2\varphi_3)}{8A \sin^2(\pi - \varphi_3)} \right) \quad (13)
\]
where $\varphi_\alpha$ is the contact angle of the $\alpha^{th}$ phase, and $A$ is the area of the liquid lens.

Based on the initial diameter of circle obtained from a diamond, equation (13) predicts a diameter of 0.415 while the result obtained from the simulation is 0.413. It is obvious in figure 4-a that the difference between theory and simulation is much greater in the case where a crude circle is used as the initial condition for the simulations. The analytical result for the crude circle is 0.406 and the simulation results in an equilibrium diameter of 0.389. It is obvious in figure 4-b that the difference between theory and simulation is much greater in the case where a crude circle is used as the initial condition for the
Having chosen the second method for generating an initial circular bubble geometry, figure 5 shows the time evolution of a fluid lens between two layers of fluid. In this case, all fluid properties are set to 1 while binary surface tension coefficients, $\gamma_{ij}$, are equal between each pair of surfaces. The time snapshots for particle positions inside the lens is also provided in figure 6.

4 Conclusions

In this study, a three-phase ISPH method is developed and presented for the simulation of the three-phase flows. Phase specific surface tension coefficient [6] is used to obtain the surface tension force for the systems with three components. The applicability of this formulations for two-phase flows is demonstrated. In addition, It is observed that choosing appropriate initial condition is crucial to obtain accurate results. And finally, it is shown that the equilibrium three-phase transverse lens diameter obtained is in good agreement with the analytical one.

5 Acknowledgement

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References


NUMERICAL SIMULATION OF OIL LEAKAGE, WATER FLOODING AND DAMAGED STABILITY OF OIL CARRIER BASED ON MOVING PARTICLE SEMI-IMPLICIT (MPS) METHOD

LIANG-YEE CHENG *, DIOGO V. GOMES † ADRIANO M. YOSHINO † AND KAZUO NISHIMOTO ‡

* Dept. Construction Engineering, Escola Politécnica
University of São Paulo
Av. Almeida Prado, Trav. 2 No. 83, Ed. Engenharia Civil, 05508-900 São Paulo, SP, Brazil
e-mail: cheng.yee@poli.usp.br, web page: http://www.pcc.usp.br

† Dept. Naval Engineering Naval Architecture and Ocean Engineering, Escola Politécnica
University of São Paulo
Av. Professor Melo Moraes, 2231, 05508-900 São Paulo, SP, Brazil
e-mail: knishimo@usp.br, web page: http://tpn.usp.br

Key words: Moving Particle Semi-Implicit, MPS, multiphase flow, oil leakage, water flooding, damaged stability.

Abstract. Oil leakage or water flooding in a damaged oil carrier are complex phenomena that involve fluid-solid interaction with complicated geometry and multiphase flow. In order to assess the damaged stability and environmental impact when the damage occurs, the present research models the non-linear hydrodynamic problems by using a numerical approach based on MPS (Moving particle Semi-Implicit) method. The comparison of numerical results with that obtained by quasi-static approach shows the limit of validity of the last one. Considering the reduced dimension of the opening of the damage, the effects of the resolution of spatial discretization are also analysed.

1 INTRODUCTION

Oil leakage or water flooding in case of damage are of great concern in the design and operation of crude oil carriers due to the safety and the environmental issues. Due to the fluid-solid interaction with complex geometry and multiphase flow, the detailed investigation of the phenomena, including the coupled transient motions of the fluids and the hull, still remains as a challenge.

Within this context, the objective of the present research is to carry out a coupled transient analysis of the oil leakage and water flooding processes and to determine the final list angles and oil leak or water flooding volumes. In order to model both the motion of the vessel and the oil-water multiphase flow with free surface, a numerical approach based on MPS (Moving particle Semi-Implicit) method [1] was adopted. On the other hand, for the surface tension in
the free surface and in the oil-water interface, as well as the wettability of the solid surfaces, an inter-particle potential force model was used [2].

For sake of simplicity, a two dimensional small scaled model and still water condition were considered and the results were compared with that obtained by the stability analysis software SSTAB, which provides the final list angle in case of the damage.

In the previous works [3,4], the dynamics of the oil leakage and water flooding process were analysed taking into account several loading conditions and heights of damage opening. The modelling of the towing tank was also improved to reduce the undesirable effects of wave reflection from the side wall of the tank to achieve more stable and accurate transient behaviours. Nevertheless, in the cases where the volume of leakage or flooding is small, the concern about the accuracy of the particle modelling still remains. This concern is especially important because of the inter-particle potential force approach that may require a higher resolution of the spatial discretization to model the oil-water interface. In this way, beside the analyses on new loading conditions, one of the objectives of the present paper is to identify the situations where the spatial resolution might be relevant to improve the accuracy of the numerical results.

2 NUMERICAL METHOD

The governing equations for the incompressible viscous flow to be solved in this study are:

Continuity equation

$$\frac{D\rho}{Dt} = -\rho(\nabla \cdot \bar{u}) = 0$$

(1)

and the momentum equation

$$\frac{D\bar{u}}{Dt} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \bar{u} + \bar{g} + \frac{\bar{\sigma}}{\rho}$$

(2)

Where, $\rho$ is density, $\bar{u}$ is velocity, $p$ is pressure, $\nu$ is kinematic viscosity, $\bar{\sigma}$ is surface tension and $\bar{g}$ is the gravity.

The Moving Particle Semi-implicit (MPS) is a Lagrangian meshless method, in which the space domain is discretized in particles, and all the differential operators are obtained from a particle interaction model based on the weight function that might be given by:

$$w(r) = \begin{cases} \frac{r_e}{r} - 1, & (r < r_e) \\ 0, & (r > r_e) \end{cases}$$

(3)

Where, $r$ is the distance between two particles and $r_e$ is the effective radius, which limits the region where the interaction between particles occurs.

Considering a scalar function $\phi$, the gradient vector and the Laplacian of the function at a particle $i$ are determined by taken into account the values of the neighboring particles $j$. Within the range $r_e$, they are given by Eq. (4) and (5), respectively:
\[
\langle \phi \rangle_i = \frac{d}{\text{pnd}^0} \sum_{i \neq j} \left[ \frac{(\phi_j - \phi_i)}{|\vec{r}_j - \vec{r}_i|^2} (\vec{r}_j - \vec{r}_i) w(|\vec{r}_j - \vec{r}_i|) \right]
\]

(4)

\[
\langle \nabla^2 \phi \rangle_i = \frac{2d}{\text{pnd}^0 \lambda} \sum_{i \neq j} \left[ (\phi_j - \phi_i) w(|\vec{r}_j - \vec{r}_i|) \right]
\]

(5)

Where, \(d\) is the number of spatial dimensions, \(\text{pnd}\) is the particle number density, \(\vec{r}_i\) and \(\vec{r}_j\) are, respectively, the position vector of particles \(i\) and its neighbor particle \(j\). \(\lambda\) is calculated by:

\[
\lambda = \frac{\sum_{i \neq j} |\vec{r}_j - \vec{r}_i|^2 w(|\vec{r}_j - \vec{r}_i|)}{\sum_{i \neq j} w(|\vec{r}_j - \vec{r}_i|)}
\]

(6)

Particle number density (\(\text{pnd}\)) is proportional to the fluid density and it is given by:

\[
\text{pnd} = \sum_{i \neq j} w(|\vec{r}_j - \vec{r}_i|)
\]

(7)

and \(\text{pnd}^0\) is the initial value of \(\text{pnd}\).

The MPS method adopts a semi-implicit algorithm. Except the pressure gradient term, the terms in the right side of Navier-Stokes equation are calculated explicitly to estimate velocity and position. After that, the Poisson's equation of pressure is solved implicitly at \((t + \Delta t)\). The Poisson’s equation is given by:

\[
\langle \nabla^2 \text{p} \rangle_i^{t + \Delta t} = -\frac{\rho}{\Delta t^2} \frac{\text{pnd}^* - \text{pnd}^0}{\text{pnd}^0}
\]

(8)

Where, \(\text{pnd}^*\) is the particle number density obtained from the particle position estimated explicitly. \(\text{pnd}^*\) is kept as \(\text{pnd}^0\) to ensure the condition of incompressibility. The term of the left hand side of equation (8) can be discretized using the Laplacian model, leading to a system of linear equations.

For the present two-dimensional analysis, \(r_c\) was set to 2.1 \(l_0\), where \(l_0\) is the initial distance between particles, to calculate pressure gradient and the particle number density. \(r_c\) is set to be 4.0 \(l_0\) for cases involving the Laplacian operator.

When the particle number density of a particle is smaller than \(\beta \cdot \text{pnd}\), it is considered to be on the free surface. The pressure of all free surface particles is set to zero. According to Koshizuka and Oka [1], \(\beta\) may vary between 0.80 and 0.99.

For the calculation of the surface tension \(\sigma\) on the free surface and at the oil-water interface, the approach proposed by Kondo et al [2] is adopted. According to the proposal of
Kondo et al [2], the surface tension, which is originated from the intermolecular forces, can be approximated by an inter-particle potential force model whose function is given by:

\[ P(r) = C \cdot p(r) \]  \hspace{1cm} \text{(9)}

where \( C \) is a coefficient that defines the intensity of the inter-particle potential, and \( p(r) \) is the shape function of the potential given by:

\[ p(r) = \frac{1}{3} (r - \frac{3}{2} r_{\text{min}} + \frac{1}{2} r_e) (r - r_e)^2 \]  \hspace{1cm} \text{(10)}

The coefficient \( C \) is obtained from the energy required to form free surfaces when particles from a domain \( A \) separate from their neighbor of another domain \( B \).

\[ C = 2 \sum_{i \in A, j \in B} \frac{r_{\text{min}}^2}{p(r_{i,j})} \sigma \]  \hspace{1cm} \text{(11)}

Finally, the force due to surface tension is determined from the spatial derivative of the potential:

\[ \frac{dP(r)}{dr} = C(r - r_{\text{min}})(r - r_e) \]  \hspace{1cm} \text{(12)}

In MPS, rows of different type of particles are used to describe the geometry of the rigid walls. Pressure is calculated in the first row that is in contact with fluids. The rows of particles that have no contact with fluids are formed by dummy particles used to guarantee the correct calculation of the particle number density, but in which the calculation of pressure is not necessary.

In case of the floating body with inner tank analyzed in the present study, as the calculation of the liquid pressure on the outside of the hull must not affect the calculation of the pressure inside the hull, and vice-versa, for \( r_e \) equals to 2.1 \( l_0 \), it is necessary put at least two rows of dummy particles between the rows of pressure particles that define the geometry of the hull and the inner tank, as shown in Figure 1.

Force and moment acting on the hull are calculated by integrating the pressure on both external and internal sides of the body. The elementary area of the wall is defined as the half distance between a hull particle and one of its neighbor particles. Each area has its normal orienting to the fluid side. Figure 2 shows an example of hull particles, their elementary areas and normal vectors.

The force on the hull and the moment applied at the center of gravity are as follows:

\[ F = \sum_i p_i \cdot (S_{i1} \cdot \vec{n}_{i1} + S_{i2} \cdot \vec{n}_{i2}) \]

\[ M = \sum_i p_i \cdot (S_{i1} \cdot \vec{n}_{i1} + S_{i2} \cdot \vec{n}_{i2}) \times (\vec{r}_i - \vec{r}_{CG}) \]  \hspace{1cm} \text{(13)}

Where, \( s_{i1} \) and \( s_{i2} \) are the dimension of the two elementary areas of particle \( i \); \( p_i \) is the pressure of particle \( i \); \( \vec{n}_{i1} \) and \( \vec{n}_{i2} \) are the normal vectors of \( s_{i1} \) and \( s_{i2} \), respectively, and \( \vec{r}_{CG} \)
is the position vector of center of gravity of the floating body.

With the force and the moment calculated by equations (13), the dynamics of the floating body can be obtained by:

\[ m \frac{d^2 \vec{r}_{CG}}{dt^2} = F \]

\[ I \frac{d^2 \theta}{dt^2} = M \]

where, \( m \) and \( I \) are mass and inertia of rigid body respectively; \( \theta \) is the roll angle.

### 3 CASES OF STUDY

To investigate the oil leakage or water flooding processes in a damaged oil carrier, a 2D numerical scaled model was used. The main characteristics of the model are described in Table 1.

<table>
<thead>
<tr>
<th>Property</th>
<th>Without ballast (B0)</th>
<th>With ballast (B15)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam (m)</td>
<td>0.415</td>
<td>0.415</td>
</tr>
<tr>
<td>Depth (m)</td>
<td>0.325</td>
<td>0.325</td>
</tr>
<tr>
<td>Mass (kg/m)</td>
<td>25.109</td>
<td>40.109</td>
</tr>
<tr>
<td>Inertia (Kgm²/m)</td>
<td>0.801</td>
<td>1.088</td>
</tr>
<tr>
<td>TCG (m)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>VCG (m)</td>
<td>0.129</td>
<td>0.094</td>
</tr>
</tbody>
</table>
The scaled model has two internal tanks. The thickness of the walls is 0.02 m except in center, where the thickness is 0.025 m, and in the bottom, where the thickness of 0.055 m is used to model the double bottom. The opening for the oil leakage is 0.05 m. In the case shown in Figure 3, the opening height is 0.20 m from the keel, and the filling ratio of the internal tank is 75%.

![Figure 3: Cross-section of the model showing the opening height of 0.20 m from the keel, and 75% filling](image)

The total width of the towing tank used in the numerical simulations is 2.7 m, as shown in Figure 4. In order to minimize the reflection of waves generated by the dynamic motion of the hull, beaches of 0.8 m are modeled in both extremity of the towing tank. The slope of the beaches is approximately 30 degrees. Squares of 3x3 particles are fixed close to the beaches. The depth of the towing tank used in the simulation is 0.40 m.

Table 2 gives the nomenclature of the cases analyzed in the present study. Three different location of damage and three levels of filling inside the tanks were considered. Due to the concern about the accuracy of the particle modelling, simulations with two levels of spatial discretization were performed for each case listed in Table 2: low and high resolutions. The simulations with low resolution were carried out by using distance between particles of 0.0050 m and there are about 34000 particles in a typical case, as in the previous works [3,4]. On the other hand, the simulations with high resolution were performed using distance between particles of 0.0025 m with near to 140000 particles in a typical case. The time step was 0.0005 s and simulation times up to 10.0 s were used.

The properties of the water and the oil are given in Table 3.

### Table 2: The cases of study.

<table>
<thead>
<tr>
<th>Case denomination</th>
<th>Filling ratio (%)</th>
<th>Damage height above the keel (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B0_75%_020</td>
<td>75</td>
<td>0.20</td>
</tr>
<tr>
<td>B0_75%_014</td>
<td>75</td>
<td>0.14</td>
</tr>
<tr>
<td>B0_75%_010</td>
<td>75</td>
<td>0.10</td>
</tr>
<tr>
<td>B0_45%_014</td>
<td>45</td>
<td>0.14</td>
</tr>
<tr>
<td>B0_45%_010</td>
<td>45</td>
<td>0.10</td>
</tr>
<tr>
<td>B0_25%_010</td>
<td>25</td>
<td>0.01</td>
</tr>
</tbody>
</table>
Table 3: The properties of the water and oil.

<table>
<thead>
<tr>
<th>Property</th>
<th>Water</th>
<th>Oil</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>1000.0</td>
<td>900.0</td>
</tr>
<tr>
<td>Viscosity (m²/s)</td>
<td>1.0x10⁻⁶</td>
<td>5.0x10⁻⁵</td>
</tr>
<tr>
<td>Surface Tension Coefficient (N/m)</td>
<td>0.072</td>
<td>0.026</td>
</tr>
</tbody>
</table>

4 RESULTS AND DISCUSSIONS

Figure 5 gives the snapshots of the animation obtained from the MPS simulation with 75% filling and opening at 0.10 m above the keel (B0_75%_010). Owing to large vertical distance from oil level to opening position, where the internal oil pressure higher than external water one, this is the case in which large oil leak is expected together with more violent transient motions. Actually, the transient analysis performed by the present study shows that a list angle nearly 30° degrees is reached in about 2 seconds after the breakdown. Also, beside the roll motion of the hull, drift motion induced by the leakage occurs in the beginning of the process when a relatively large volume of the oil is released suddenly. The comparison between Figure 5(a) and Figure 5(b) shows that the higher spatial resolution gives more detail description of the oil flow outside of the hull.

The validation of final equilibrium angle of list has been carried out by using SSTAB [5]. SSTAB uses hydrostatic theory to calculate the stability of floating bodies with and without free surface effects, and free to pitch and heavy. In order to model the 2D problem, a 3D model of B/L=1/100 with constant cross section and without trim is used in the SSTAB
calculations. Although SSTAB is able to provide an estimate the final list angle through a quasi-static approach, it is unable to take into account the dynamic effects due to oil leakage or water flooding. In this way, the final list angle provided by SSTAB is determined by using the volume obtained by MPS simulation.

Figure 6(a) provides the comparison of the time series of the roll motions obtained by MPS simulation with low and high resolutions, together with the final list angles obtained by SSTAB for the case B0_75%_010. The transient motions calculated by MPS show damped oscillations of the motion after quick inclination from the initial position. Despite more detail description of the oil flow outside the hull provided by the simulation with high resolution, the agreement between the time series of the low and high resolutions is very good. This is because the details of the oil flow outside the hull are not relevant for the hull motion and the refinement of the spatial resolution has no effect on the numerical results.

In the case of B0_75%_014 (Figure 6(b)), in which the leakage volume and final list are smaller than the former one, the same tendency is observed in despite of the slightly larger discrepancy between the motion time series obtained by the simulations with low and high resolutions. In addition to this, the computed time series of both B0_75%_010 and B0_75%_014 converge to mean values that agree very well with the final list angles obtained by SSTAB.

![Figure 6](image)

**Figure 6**: Comparison of the time histories of the list angle obtained by transient analysis of MPS and list angle obtained by the hydrostatic analysis of SSTAB showing the effects of resolution in the cases B0_75%_010 (a) and B0_75%_014 (b)

Figure 7(a) and Figure 7(b) show the time series of the cases B0_45%_010 and B0_45%_014, respectively. As in the cases with 75% filling, oil leakage occurs. However, as the initial vertical distances between the oil level and the opening are decreased, both the leakage volume and the final list angles are reduced. This might be the reason why the discrepancies between the time series with low and high resolutions occur from the early instants of the simulations.

The snapshots of B0_45%_014 presented in Figure 8 show that this is a critical case were very small volume of oil is released and spatial resolution of MPS modeling might affect small simulation results. Also, the drift motion becomes negligible and there are almost no dynamic effects induced by the a relatively small volume of oil leakage.
Figure 7: Comparison of the time histories of the list angle obtained by transient analysis of MPS and list angle obtained by the hydrostatic analysis of SSTAB showing the effects of resolution in the cases B0_45%_010 (a) and B0_45%_014 (b).

Figure 8: Snapshots of the simulations of the case B0_45%_014 with low (a) and high (b) resolutions.

Figure 9 gives the volume of the oil leakage calculated by MPS, together with the leakage estimate by using SSTAB through quasi-static approach. The vertical axis of Figure 9 is the volume of the leaked oil in relation to the volume of one internal tank. The comparison between the results shows very good agreement. Despite the dynamic effects such as roll and drift motions, the discrepancies are quite small, especially in the cases where the leakage is larger. On the other hand, similar tendency can be observed in the discrepancies between the low and high resolution results. For the case B0_45%_014, for example, in which the leakage
is about 8%, the discrepancy due to the spatial resolution achieves 17.5%.

![Figure 9: Oil leakage obtained by MPS and by quasi-static calculation using SSTAB for 45% and 75% filling and opening height of 0.10 m, 0.14 m and 0.20 m](image)

Also, as shown in Figure 9, for filling ration of 25% (B0_25%), the quasi-static approach predicts oil leakage when opening height is 0.10 m. This occurs because one of the key assumptions of the quasi-static approach is very small opening. However, as illustrated in Figure 10, which presents the snapshots of the simulation results of B0_25%_010, instead of oil leakage, water flooding occurs.

Figure 10 clearly shows how this situation unexpected by quasi-static approach occurs: initially, as the oil and water surface and the opening are almost at same level, after a very shortly oil leakage, increasing volume of water floods into the tank. As the negative list angle increases, water floods quickly into the tank and the final list angle reaches to -45°. Finally, the flooding water, whose density and surface tension are larger than oil, washes the bottom and inner side walls of the tank and pushes the oil to the tank ceiling. As the void space of the tank is relatively large in this case, a huge amount of water floods into the tank and the final volume of flooded water calculated by MPS is as large as 65.3% of the volume of one internal tank. This huge discrepancy between the results obtained numerical and analytically shows the limit of the validity of the quasi-static approach.

Time series of the cases B0_25%_010 is illustrated in Figure 11. The figure shows that the transient motion is strongly affected by the spatial resolution: the roll motion obtained with higher spatial resolution is faster than that obtained with low resolution. As shown in Figure 10, the oil and water flows through a small portion of the opening. In the simulation with low resolution the computed inward and outward flows are smaller because it involves few fluid particles, and most of them are the free surface one, without dynamic pressure.
Figure 10: Snapshots of the simulations of the case B0_25%_010 with low (a) and high (b) resolutions

Figure 11: Comparison of the time histories of the list angle obtained by transient analysis of MPS and list angle obtained by the hydrostatic analysis of SSTAB showing the effects of resolution in the cases B0_25%_010

5 CONCLUDING REMARKS

In the present paper, a numerical approach based on MPS (Moving particle Semi-Implicit) method is adopted to model the fluid-solid interaction with complex geometry and multiphase oil-water flow to investigate the dynamics of the oil leakage and water flooding in a damaged
crude oil carrier.

The numerical simulations of the transient motion show that the drift motion induced by the leakage may occur in the beginning, when a relatively large volume of oil is released suddenly. From the comparison of the final list angles with that obtained by SSTAB, which is a static stability code, it is clear that the numerical approach is very effective to predict the dynamic behavior of a damaged oil carrier from breakdown to final list, such as damped roll motion and its response time, which might be important for the safeguard issues.

Concerning the accuracy of the numerical results, it increases in cases where the filling ratio is large and the height of the damage is low. The effects of the spatial resolution of the MPS modeling on the accuracy of the numerical results were also analyzed, and it is critical in the case of low filling where the water flooding occurs or when leakage volume is small.

On the other hand, despite the complete simulation of the oil spillage was not realized because the formation of a thin film of oil will demand a very large number of particles that is beyond the scope of the present study, the comparison of the computed oil volume with that obtained by quasi-static approach shows the limit of validity of the last one.

Finally, for sake of simplicity, 2D modeling was carried out to investigate the complex fluid-solid interaction phenomena. This is a hypothetical situation in which the dimension of the damage is much larger than the actual cases. In this way, instead of extrapolating straightforwardly the 2D results to the actual situations, further complete 3D analysis should be done. In addition to this, future works on the effects of the air inside the tank are also required.

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REFERENCES

PERMEABILITY ASSESSMENT OF HETEROGENEOUS POROUS MEDIA USING THE LATTICE BOLTZMANN METHOD

B. Jones, Y. T. Feng

Civil and Computational Engineering Centre
College of Engineering, Swansea University
Swansea, SA2 8PP, UK
email: 403113@swan.ac.uk

Key words: Lattice Boltzmann, Material Characterisation, Permeability, Partial Bounce-back

Abstract. Material characterisation is one of the most important aspects of accurate numerical modelling; correct material properties must be obtained for the correct behaviour to be observed. Traditionally permeability is measured by applying a constant/falling head test to a material sample, where such tests may involve many samples at varying pressure gradients. However current X-Ray micro-tomography techniques allow us to avoid physical lab tests by providing the ability to reproduce a voxelised representation of the internal structure of a porous medium. The Lattice Boltzmann Method may then be used to model a pressure induced flow field within the sample so that permeability may be numerically approximated. Typically this process is carried out after a thresholding procedure has been applied to the voxelised geometry to split it into definite solid and void spaces, at the expense of accurate representation of the geometry. In an attempt to better represent the porous medium the Immersed Moving Boundary technique was applied in such a way that it partially applies the bounce back boundary condition so that the strength of this application scales with the porosity of a given lattice node. This allows us to consider directly raw voxel values, avoiding the need for any thresholding procedure. To validate this hypothesis two test cases were explored in 2D; flow past a periodic array of cylinders by use of a unit cell model, and flow through a simple heterogeneous porous medium. Results were compared with analytical expressions where available, and published expressions for permeability evaluation of porous media. Results were found to be in good agreement with the available expressions.

1 INTRODUCTION

Accurate assessment of material permeability is a challenge encountered by many industrial organizations, in particular those engaged in Oil and Gas production. When such
an organization requires knowledge of material permeability, they must gather a set of samples of sufficient size and submit them to a laboratory where a constant head test may be applied to assess permeability. Such tests may be destructive and time consuming, adding cost to an operation. It would be easy to assume that gathering samples is cheap; however if one considers the fact that these organizations may typically require knowledge of the permeability of rock which exists kilometres below the earth’s surface, then it may also be seen that gathering material samples is in itself an extremely costly venture. In order to gain access to rock material at such depth a borehole must be drilled, and drilling must then be interrupted as and when material samples are to be extracted. This procedure operates on the assumption that the cuttings produced during drilling are too small to be subjected to traditional laboratory scale testing. It is therefore desirable to develop alternative means of permeability evaluation which are able to consider drill cuttings, the gathering of which has no impact on the drilling schedule of a borehole.

The Lattice Boltzmann Method\(^1\) (LBM) has become a popular method in the field of porous media flow modelling,\(^2,3\) in large part due to the simplicity of constructing a lattice which may represent heterogeneous porous media. Since the LBM operates on a regular lattice, in most cases a square lattice, one can avoid the complexities of meshing routines required by more traditional methods such as the Finite Volume or Finite Element methods. The LBM was originally derived from the Boltzmann equation, which describes the statistical likelihood that a particle exists at any given point in space and time with a given momentum. In the LBM, space and momentum are discretized so that particles may exist only at specific points with momentum aligned to a given set of vectors. The method is computationally cheap and efficient and may be parallelized with ease. Interaction between a fluid and a solid within an LBM model can be easily accounted for by use of what is known as the bounce back boundary condition, an extremely simple boundary condition which serves only to reflect any momentum incoming to the boundary. Within an LBM model any particular computational node, or lattice node, may have the bounce back condition imposed upon it. The result of the bounce back boundary is an almost no-slip condition at the interface between a bounce back node and a fluid node. The bounce back boundary condition therefore provides the ability to simply represent what may be a complex geometry, though its use does bring a significant drawback in so far as curved and inclined boundaries can only be represented using a staircase approximation.

X-Ray Micro-tomography (micro-CT) provides the ability to determine the internal micro structure of rock samples, and the LBM represents a suitable method for modelling the flow of fluids through this micro structure. A micro-CT scan of a rock sample would return a voxelised representation of the rock micro-structure, previous studies in this field have applied a thresholding procedure\(^3\) to the voxelised geometry so that the bounce back condition may be applied to represent the rock medium. The goal of this study is to explore a way to avoid this thresholding procedure by novel use of the Immersed Moving Boundary method for LBM\(^4\) in order to directly consider the voxelised geometry produced by a micro-CT scan, so that material permeability may be numerically approximated.
The use of the LBM, and aforementioned boundary conditions, with respect to permeability analysis was explored with a series of 2D test cases. These test cases include flow past a periodic array of hexagonally packed cylinders, flow through a homogeneous porous medium and flow through a simple heterogeneous porous medium.

2 PERMEABILITY ASSESSMENT

This section details methods by which the permeability of a porous medium may be analysed, both physically and computationally. In both physical and computational testing Darcy’s equation is employed:

$$q = -\frac{k}{\mu} \nabla P$$

which includes terms for flux, $q$, viscosity, $\mu$, pressure gradient, $\nabla P$ and finally material permeability, $k$ in which we are interested. Darcy’s equation defines a linear relationship between the flux, $q$, and pressure gradient, $\nabla P$.

2.1 Physical Testing

A typical technique employed to assess the permeability of a material sample is the constant head test. The constant head test exploits the relationship between fluid flux, an applied pressure gradient and material permeability, as defined by Darcy’s equation (1). When carrying out a constant head test on a material sample, the sample is initially saturated with fluid, a pressure gradient is then applied across the sample and the resultant volumetric flow rate is measured. Since the fluid viscosity is known, a known pressure gradient is applied, and the volumetric flowrate can be measured, Darcy’s equation may then be used to calculate the permeability of the material sample.

2.2 Computational Testing

Computational permeability analysis is carried out with an identical methodology to physical permeability analysis. If the internal micro structure of a porous medium is known, it may be reproduced in a computational domain; using current CFD technology, in this case the LBM, one can then impose a pressure driven flow upon a computational domain. The fluid flux through this domain may be approximated by inspection of the results of the modelled pressure driven flow and, as long as the model parameters define a case where the modelled fluid is of known viscosity, the permeability of the modelled sample may be approximated.

3 NUMERICAL TECHNIQUE

The numerical techniques employed in this study are detailed and explained within this section, including the standard Lattice Boltzmann formulation, the simple bounce back no slip condition, and an Immersed Moving Boundary technique. A brief description of
the Zhou/He boundary condition\textsuperscript{5} is also included as it is used in this study to impose a pressure gradient upon the considered computational domains.

3.1 The Lattice Boltzmann Method

The standard DdQ\textsubscript{9} Lattice Boltzmann scheme with an LBGK collision term\textsuperscript{6} operates on a \(d\)-dimensional square lattice of lattice nodes connected by \(q−1\) vectors. Since this study is concerned with 2D test cases only the D2Q9 lattice node was used, a diagram of which shown in Fig. 1. The D2Q9 lattice, and indeed any compatible lattice, consists of evenly spaced lattice nodes separated by a distance, \(h\), in every dimension. Each lattice node is connected to its neighbours by 8 vectors, \(\mathbf{e}_i\), and each vector has a particle distribution function (PDF), \(f_i\), associated with it along with a ninth ”rest” PDF. If the numbering convention applied to the lattice node shown in Fig. 1 is respected, the corresponding vectors, \(\mathbf{e}_i\), are given by:

\[
\begin{align*}
\mathbf{e}_0 & = (0, 0) \\
\mathbf{e}_i & = C \left( \cos \frac{\pi(i-1)}{2}, \sin \frac{\pi(i-1)}{2} \right) \quad (i = 1, \ldots, 4) \\
\mathbf{e}_i & = C \left( \cos \frac{\pi(2i-9)}{4}, \sin \frac{\pi(2i-9)}{4} \right) \quad (i = 5, \ldots, 8)
\end{align*}
\]

in which the lattice speed, \(C\), is related to the distance between the lattice nodes, \(h\), and the discrete lattice time step, \(\Delta t\),

\[
C = \frac{h}{\Delta t}
\]
The evolution of these PDF’s is defined by the LBGK Lattice Boltzmann equation:

\[ f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = \frac{1}{\tau}(f_{eq}^i(\rho, \mathbf{u}) - f_i(x, t)) \] (4)

where the additional terms, \( \rho \), \( \mathbf{x} \) and \( \tau \) are respectively the fluid density, position and relaxation time of a given lattice node. The relaxation time is a non-dimensional control parameter of a Lattice Boltzmann model, and defines the strength of the LBGK collision process which represents a relaxation to some equilibrium state. In terms of the LBM, the equilibrium state is defined by the equilibrium particle distribution function,

\[ f_{eq}^i = \omega_i \rho \left( 1 + \frac{3}{C^2 e_i \cdot \mathbf{v}} + \frac{9}{2C^4} (e_i \cdot \mathbf{v})^2 - \frac{3}{2C^2} \mathbf{v} \cdot \mathbf{v} \right) \] (5)

in which the weighting factors, \( \omega_i \), are:

\[ \omega_0 = \frac{4}{9}, \quad \omega_{1,2,3,4} = \frac{1}{9}, \quad \omega_{5,5,6,8} = \frac{1}{36} \] (6)

The macroscopic values of density, \( \rho \), and momentum, \( \rho \mathbf{u} \), can be calculated for each lattice node by,

\[ \rho = \sum_i f_i \] (7)

\[ \rho \mathbf{u} = \sum_i e_i f_i \] (8)

respectively. The pressure, \( P \), is related to the density, \( \rho \), as:

\[ P = C_s^2 \rho \] (9)

where the lattice speed of sound, \( C_s \), is:

\[ C_s = C/\sqrt{3} \] (10)

Also, the fluid viscosity is related to the parameters in LBM as:

\[ \nu = \frac{1}{3} \left( \frac{\tau}{2} - \frac{1}{2} \right) \frac{h^2}{\Delta t} \] (11)

Equation (4) dictates an evolution procedure for the PDF’s that can be split into two stages; streaming, represented by the left hand side of the equation; and collision, represented by the right hand side of the equation. The collision step in this formulation is an LBGK collision process which, as stated, represents a relaxation towards an equilibrium state. The streaming step serves only to propagate PDF’s from the lattice node in question, to its nearest neighbours. As can be seen, any numerical computation occurs only in
the collision stage; furthermore for any given lattice node operating under the standard LBM scheme all computations are purely local. In terms of computational implementation the streaming step is in its simplest form a memory transfer operation, where PDF’s are passed from one location in memory to another. Based on this it should be clear that the LBM for single phase fluid flows lends itself very well to parallel processing.

3.2 No Slip - Bounce Back

The No-Slip boundary condition is fundamental to fluid mechanics, and it implies that fluid in contact with a solid surface will travel at a velocity equal to the velocity of the surface. Due to the nature of the LBM, imposing a fixed velocity, or density, at a point in space is non-trivial. Equation (8) relates the effective momentum at a lattice node to its PDF’s, so to fix the velocity at any given lattice node the relationship defined by this equation must be preserved. Unfortunately since equation (8) is the only equation available relating the PDF values to momentum, calculation of the required PDF values to fix the velocity at a lattice node results in this single equation with 9 unknowns. This problem however can be avoided through the use of what is known as the bounce back boundary condition.7

In an LBM model a solid surface may be represented by a bounce back node, or series of bounce back nodes. When a lattice node is deemed bounce back then any momentum incoming to the lattice node is reflected back towards the lattice node it came from in the subsequent time step, with no collision process occurring on the bounce back lattice node. This operation ultimately modifies the evolution equation for the lattice node in question to read as equation (12).

\[ f_i(x + e_i \Delta t, t + \Delta t) = f_{-i}(x, t) \]  

(12)

where \( f_{-i} \) is the PDF who’s associated vector points in the opposite direction to the PDF \( f_i \).

Due to the simplicity of the bounce back boundary condition, its use is convenient but not ideal. He et al. showed that use of the bounce back boundary condition in an LBM model will degrade the accuracy of the model to first order in space.7

3.3 No Slip - Partial Bounce Back

The Partial Bounce Back (PBB) boundary condition refers to a specific use of the Immersed Moving Boundary (IMB) condition proposed by Noble & Torczynski.4 The IMB condition is one which attempts to incorporate the interaction between a fluid and a solid body moving through it. An IMB may represent a boundary that does not conform to the computational grid, or lattice in this case, and this boundary may be moving with some velocity relative to the surrounding fluid. It can be seen in Fig. 2 that an object which does not conform to the computational lattice may only partially occupy any given lattice node; this may well be the case when considering a non-integer voxel taken from a
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micro-CT scan of a rock medium representing a definite fluid solid boundary intersecting the voxel. The IMB technique proposed by Noble & Torczynski results in a modification to equation (4) to read as:

\[ f_i(x + \epsilon_i \Delta_t, t + \Delta_t) - f_i(x, t) = [1 - B(x, \epsilon_s)] \Omega_i^{BGK} + B(x, \epsilon_s) \Omega_i^S \]  \tag{13}

where,

\[ \Omega_i^{BGK} = \frac{1}{\tau}(f_i^{eq}(\rho, u_f) - f_i(x, t)) \]  \tag{14}

and,

\[ \Omega_i^S = f_{-i}(x, t) - f_i(x, t) + f_i^{eq}(\rho, u_s) - f_{-i}^{eq}(\rho, u_f) \]  \tag{15}

or,

\[ \Omega_i^S = f_{-i}(x, t) - f_i(x, t) + f_i^{eq}(\rho, u_s) - f_{-i}^{eq}(\rho, u_f) \]  \tag{16}

in which \( f_i^{eq}(\rho, u_s) \) and \( f_i^{eq}(\rho, u_f) \) are the equilibrium particle distribution functions as given by equation (5) with \( u = u_s \) and \( u = u_f \) respectively. \( u_s \) is the velocity of the boundary, and \( u_f \) is the velocity of the fluid.

Equation (15) is the expression originally proposed for \( \Omega_i^S \); though another expression, equation (16), was proposed by Holdych\(^8\) which has been shown to increase the accuracy of computed force and torque on a sphere in poiseuille flow when compared with the original expression.\(^9\) In the interests of completeness both expressions were explored in this study with respect to the accuracy of measured permeability.

In equation (13), \( B(x, \epsilon_s) \) is a function which represents a solid fraction field across the domain allowing for a different solid fraction, \( \epsilon_s \), at individual lattice nodes. In the original paper Noble & Torczynski propose two formulations for \( B(x, \epsilon_s) \); the first is direct use of solid fraction so that

\[ B(x, \epsilon_s) = \epsilon_s(x) \]  \tag{17}

The second formulation is a function of \( \epsilon_s \) with relaxation time dependent weighting

\[ B(x) = \frac{\epsilon_s(x)(\tau - 1/2)}{(1 + \epsilon_s(x)) + (\tau - 1/2)} \]  \tag{18}

which is reported to work well for \( \tau \) between 0.6 and 0.9. Though the impact of the relaxation time dependent weighting is negligible, and was shown not to impact upon results.\(^10\) Therefore the simpler form of \( B(x, \epsilon_s) \) given by equation (17) was used in this study.

The effect of this modification to the Lattice Boltzmann Equation is essentially the partial application of the bounce back boundary condition to every lattice node. The strength of this partial application is dependent upon the velocity of the boundary, and the proportion of a lattice node which is occupied by the boundary, or porosity. This form of the PBB condition has previously been used by Feng et al. who have shown it
Figure 2: An example of a boundary which does not conform to the computational grid to be a suitable choice for considering the interaction between the flow of a fluid and immersed objects in both 2D\textsuperscript{10} and 3D.\textsuperscript{11} Using such a boundary condition with the boundary velocity set to zero leaves us with the partial application of the bounce back condition scaling only with porosity. In this way, the proposed boundary scheme may be used to consider intrinsically porous lattice nodes. The relationship between resultant permeability and imposed porosity using the PBB condition with a zero boundary velocity was explored and results are presented in section 4.1.

The PBB condition allows for direct consideration of non-integer micro-CT voxels. Where a non-integer voxel would represent either a definite fluid/solid boundary or an intrinsically porous region of the medium, the ability of the PBB condition to consider such regions was explored in two tests models designed to represent each case.

### 3.4 Applied Pressure Drop

In order to use Darcy’s equation to numerically approximate material permeability, a pressure gradient must be applied across the considered computational domain. To do this in the LBM model, the popular Zhou/He boundary condition has been used.\textsuperscript{5} As has been stated, imposition of a specific value of density, pressure or momentum on any one lattice node is non-trivial. This is due to the fact that for the LBM there exists only one equation linking the desired macroscopic value to the microscopic PDF’s, and since there are nine PDF’s for a D2Q9 lattice we are left with one equation and 9 unknowns. In an attempt to circumvent this situation Zhou & He suggested two assumptions:
• A PDF who’s origin is from within the computational domain is of the correct value.

• A PDF who’s origin is outside the boundary may be computed if the relationship proposed in equation (19) is respected for the PDF normal to the boundary (in this case \( f_1 \) is normal to the boundary).

\[
f_1 - f^{eq}_1 = f_3 - f^{eq}_3
\]  

(19)

If the stated assumptions are respected then one can apply some algebra to the LBM equations to gain expressions for the remaining non-normal PDF’s which are streamed from outside the boundary. For straight boundaries Zhou & He demonstrate second order accuracy with their boundary technique on a D2Q9 lattice. The Zhou/He boundary condition can be used to specify pressure at both the inlet and the outlet of the computational domain. With differing inlet and outlet pressure imposed, a pressure gradient across the domain will establish itself as steady state is achieved.

4 RESULTS

To test the validity of using the PBB condition to model flows which include geometry that is either porous or partially occupying lattice nodes, such as may be gained from a micro-CT scan, two test cases were explored. These test cases were flow through a periodic array of hexagonally packed cylinders, demonstrating the method’s ability to deal with lattice nodes partially occupied by a solid body; and flow through a simple heterogeneous porous media, demonstrating the method’s ability to deal with porous bodies. The relationship between the porosity of a lattice node and its permeability was also explored. A description of the tests and commentary on results is included in this section.

4.1 Relationship Between Porosity and Permeability using the PBB condition

The PBB condition was used in this study to impose an intrinsic porosity upon individual lattice nodes within a computational domain. This novel use of the technique proposed by Noble & Torczynski requires first that the relationship between the porosity and permeability of a lattice node be defined. Since no equation was available to relate these factors an experiment was carried out. The experimental set up uses the PBB condition to consider a domain of uniform porosity, Zhou/He pressure boundaries were used to impose a pressure drop between the inlet and outlet of the domain, and the resultant flow rate was measured. From this a specific value of permeability can be calculated using Darcy’s equation (1) to match a specific value of porosity. Different value’s of porosity were tested from 0.05 to 0.95 in increments of 0.05. A plot of porosity versus permeability is included in Fig. 3 which shows an exponential relationship between porosity and permeability. In the interest of simplicity all tests were carried out with \( \tau = 1 \) and a fixed arbitrary pressure drop of 0.0005, the domain consisted of 100 lattice nodes in x and y.
4.2 Unit Cell Cylinder

The Unit Cell cylinder test is designed to test the accuracy of the PBB condition with respect to permeability of a domain where the PBB condition is used to consider nodes which are intersected by a definite fluid/solid boundary. The unit cell model is representative of a periodic array of hexagonally packed cylinders and a diagram of the unit cell geometry is included in Fig. 4.

To represent the cylinder geometry using the traditional bounce back technique would leave the cylinder under defined in a 'staircase' approximation, where the curve of the cylinder edge is staggered as it passes through individual lattice nodes. Those lattice nodes whose centre is within the cylinder radius are deemed bounceback, whereas those lattice nodes whose centre is outside of the cylinder radius are simply fluid lattice nodes. This leaves the cylinder under defined as under this approximation to the cylinder surface there would be lattice nodes which are partially intersected by the cylinder surface where the centre of the lattice node in question lies outside the cylinder radius. Such lattice nodes may be accounted for by using the PBB boundary condition taking into consideration the fraction of these lattice nodes which is occupied by the cylinder.

The permeability of a periodic array of hexagonally packed cylinders was independently studied by both Gebart\textsuperscript{12} and Lee & Yang\textsuperscript{13} who have proposed expressions for permeability normalised against the cylinder diameter. Equation (20) is the expression proposed by Gebart, while equation (21) is the expression proposed by Lee & Yang.
Figure 4: Geometry of Unit Cell Cylinder

\[
\frac{k}{d^2} = \frac{4}{9\pi \sqrt{6}} \left( \sqrt{\frac{\pi/2\sqrt{3}}{1 - \phi} - 1} \right)^{5/2}
\]

(20)

\[
\frac{k}{d^2} = \frac{\phi^3(\phi - 0.2146)}{31(1 - \phi)^{1.3}}
\]

(21)

For the unit cell cylinder test the expressions proposed by Gebart and Lee & Yang are used as a benchmark against which to compare numerical results. The LBM was tested with three alternate boundary conditions to represent the cylinder geometry, bounce back, PBB with Noble & Torczynski’s original expression for \( \Omega^* \), and PBB with Holdych’s expression for \( \Omega^* \). As with the experiment investigating the relationship between lattice node porosity and permeability, the Zhou/He pressure boundary was used at the inlet and outlet to impose a pressure drop of 0.0005 across the domain with \( \tau = 1 \). Numerical results were gained for two independent cases. The first test case was a series of models at a fixed resolution of 100 lattice nodes in x and y, with varying cylinder radius. This test was designed to evaluate the accuracy of the LBM using these boundary conditions across the range of possible porosities for the model. The second test case included a series of models with a fixed cylinder radius but varying resolution, that is the ratio between radius and resolution in lattice units was fixed; designed to evaluate the sensitivity of this technique to resolution. For the test case considering varying resolution the radius was fixed such as to give porosity of the model \( \approx 0.65 \). For all test models a pressure drop is imposed, the resultant flux is measured, and the permeability is calculated using Darcy’s equation (1).

Fig. 5 shows the results of the unit cell cylinder test for varying cylinder radius. The plot of diameter normalised permeability versus porosity shows that in the low ranges of
Figure 5: Results for Unit Cell Cylinder Model with Variation of Porosity

(a) Variation of $K/d^2$ with Porosity

(b) Difference between numerical results and Gebart’s Expression

(c) Difference between numerical results and Lee & Yang’s Expression
porosity, the results match closely to the expression proposed by Lee & Yang, as porosity increases, the results begin to agree more closely with Gebart’s expression. Overall good correlation has been achieved between the numerical results and published expressions. The plots of percentage difference show that in general the results from the models using the PBB boundary condition agree more closely with the published expressions than the results gained from models using the traditional bounce back technique. Inspection of Fig. 5a also shows that although the variation of difference between the numerical results and the published expressions in figures 5b and 5c is in many cases large (> 10%), the numerical results agree more closely with the published expressions than the expressions agree with themselves.

One point of interest from these results is that when using the PBB condition with Noble & Torczynski’s original expression for \( \Omega^s \) the models exhibit some odd behaviour. For the most part, models were terminated when the root mean square of the sum of the change in velocity between time steps is sufficiently small, too ensure good results the threshold for this value was set to \( 10^{-10} \). However at high porosity, using Noble & Torczynski’s original expression for \( \Omega^s \) the root mean square of the sum of the change in velocity between time steps never fell below the threshold value.

Fig. 6 shows the results of the unit cell cylinder test for varying resolution. The plot demonstrates that up to a domain length of 200 lattice nodes in x and y, results can vary by a relatively large degree, after this point the dependence of results on domain resolution starts to become marginal as they begin to converge.

### 4.3 Simple Heterogeneous Porous Media

The simple heterogeneous porous media test is designed to evaluate how accurately the PBB condition is able to consider a medium which is completely and non-uniformly
porous. The test represents a simplified version of the case where a non-integer voxel from a micro-CT scan is the result of an area with intrinsic porosity, as opposed to a definite fluid/solid boundary. The computational domain to be considered is one which contains two regions of differing porosity, and thus permeability. Two such computational domains were used, one where these regions were aligned in parallel in the direction of flow, and one where these regions were aligned in series in the direction of flow. A diagram of this set up is included in Fig. 7.

Analytical expressions exist by which the effective permeability can be calculated if the permeability of the individual regions is known. Analytical expressions for effective permeability of such simple media can be derived for both the medium in series and in parallel. If \( h_j \) is the width or height of a permeability region, and \( k_j \) is the corresponding permeability of this region, then the effective permeability of the region may be found as,

\[
\text{Series: } k_{eff} = \frac{\sum_{j=1}^{n} h_j}{\sum_{j=1}^{n} \frac{h_j}{k_j}} \tag{22}
\]

\[
\text{Parallel: } k_{eff} = \frac{\sum_{j=1}^{n} h_j k_j}{\sum_{j=1}^{n} h_j} \tag{23}
\]

For this test the models were set up so that a pressure drop is applied between the inlet and outlet the domain using the Zhou/He pressure boundary condition as with the other test cases. The resultant flowrate is measured and the permeability is again calculated using Darcy’s equation (1). The models in series and in parallel were tested against increasing permeability difference between the two regions, where the maximum permeability difference is the case when region one has a porosity of 0.05 and region two has a porosity of 0.95. The results of this test are shown in figures 8 and 9 for the medium in series and in parallel respectively.

The results for the heterogeneous porous medium in series show excellent agreement...
Figure 8: Results for Simple Heterogeneous Porous Media Model Aligned in Series

Figure 9: Results for Simple Heterogeneous Porous Media Model Aligned in Parallel
between the numerical and analytical effective permeability, with an almost constant error of \( \approx 1\% \). The results for the heterogeneous porous medium in parallel are almost as good as for the medium in series, where the error for the smallest permeability difference being \( \approx 1\% \) and the error for the largest permeability difference being \( \approx 5\% \).

5 CONCLUSION

The goal of this study was to test the PBB boundary condition and assess its ability to deal with the type of geometry that would be gained from a micro-CT scan of porous rock. To this end the relationship between lattice node porosity and permeability was explored and reported. The PBB condition was then used to evaluate two test cases; flow past a periodic array of cylinders, and simple heterogeneous porous media. It was found that the PBB boundary condition is capable of considering boundaries which do not conform to the computational grid more accurately than if the standard bounce back boundary condition is used to represent these boundaries. In addition to this it was also shown in this test that Holdych’s expression for \( \Omega^* \) is indeed more accurate than Noble & Torczynski’s original expression. It has also been shown that the PBB boundary condition is able to accurately predict the effective permeability of simple heterogeneous porous media with a maximum error of 5\%. These facts lead us to the conclusion that the PBB boundary condition is a suitable choice for modelling the flow through a voxelised representation of the internal micro structure of a rock, while maintaining the definition of the geometry as determined by a micro-CT scan. Further work will explore the presented test cases in 3D, and ultimately lead to computational analysis of real rock geometries.

REFERENCES


SMOOTHED PARTICLE HYDRODYNAMICS SIMULATION OF NON-SPHERICAL PARTICLE SUSPENSIONS

PIT POLFER*, ANDREAS WONISCH AND TORSTEN KRAFT

Fraunhofer Institute for Mechanics of Materials IWM
Wöhlerstraße 11, 79108, Freiburg, Germany
www.en.iwm.fraunhofer.de
* corresponding author. E-mail: pit.polfer@iwm.fraunhofer.de

Key words: Suspension, SPH, Particle orientation, Tape casting

Abstract. Particulate suspensions are used in many technical areas: ceramic processing, powder metallurgy and pharmaceutical applications being only a few examples. In many of these applications the microstructure determines the product quality. To further optimize the production processes a better understanding of the rheological behavior and the microstructure development inside the suspension is needed. Therefore, a direct numerical simulation method taking into account both particle interactions and hydrodynamics has been developed. It is used to investigate the particle orientation during the tape casting of thin ceramic sheets.

1 INTRODUCTION

The rheological behavior and microstructure of a suspension are very important parameters in processes involving suspensions. E.g. in ceramic sheets produced by tape casting [1] an anisotropic micro-texture can be observed: The powder particles in the green tape are aligned in the casting direction [2]. This leads to subsequent undesired anisotropic sintering shrinkage in the later processing of the sheet. The cause for this particle orientation is the shearing of the ceramic slurry below the blade. This has recently been numerically investigated on a macroscopic scale [3].

In order to fully describe and understand such a system, not only a macroscopic but also a microscopic computational fluid dynamics model with fluid-solid coupling as well as the interaction between the particles is needed. As the length scales of the process reach over multiple magnitudes, a multi-scale approach is required. In this paper, the microscopic model and results concerning the motion of non-spherical particles in shear flow will be presented. The macroscopic model can be found in a previous paper [3].

Rigid objects composed of multiple constrained sub-particles have been used in different particle-based, meshfree methods, e.g. the Discrete Element Method (DEM) [4,5] and Dissipative Particle Dynamics (DPD) [6]. As the Smoothed Particle Hydrodynamics (SPH) [7] method is in its main features, e.g. particle-based and meshfree, similar to these it allows an easy implementation of the aforementioned concept for rigid objects. The main features of the model are given in this paper, a more detailed description can be found in [8]. Similar SPH models were published by other groups [9, 10].
2 SIMULATION MODEL

2.1 SPH Implementation

A detailed explanation of SPH used in this paper can be found in Monaghan’s review [11]. Therefore, only the basic details of SPH will be described here. SPH is a Lagrangian meshfree method to simulate fluid flows. The fluid is discretized by particles which move with the flow. The particles are not real physical entities but a mathematical form to describe the continuum. Field properties such as density, shear rate, etc. can be calculated through interpolation over the particles. This is done by using a kernel interpolation function with a given range, the so-called smoothing length. The equation for the movement of the particles is derived from the Navier-Stokes equation. In this paper the following formulation is used [12]:

\[
\frac{dv_i}{dt} = -\sum_j m_i \left( \frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \nabla W_{ij} + \sum_j m_j \left( \frac{T_{ij}}{\rho_j^2} + \frac{T_{ji}}{\rho_i^2} \right) \cdot \nabla W_{ij} + F_i
\]

where \( v_i \) is the velocity of particle \( i \) (\( i = 1 \ldots N \) , \( N \) : number of particles), \( m_i \) its mass, \( p_i \) its hydrostatic pressure, \( \rho_i \) its density, \( T_i \) the viscous stress tensor at the location of particle \( i \) and \( F_i \) a body force per unit mass for particle \( i \). \( W_{ij} \) is the kernel interpolation function between particles \( i \) and \( j \). A cubic spline kernel function and density summation formalism for the continuity equation were used.

2.2 Solid-Fluid Coupling

A rigid body is formed by a constrained cluster of SPH particles. The motion of a rigid body is governed by the summation of all forces on the SPH particles composing the rigid body. In our case these are the standard SPH forces, derived from equation (1). A rigid body motion solver [13] was implemented in our SPH code SimPARTIX.

As there is no contact force other than the SPH forces, overlap in the range of the smoothing length might occur between SPH particles of different rigid bodies. This should influence the results only slightly as the systems we investigate have low particle volume fractions and low Reynolds numbers. In this regime the viscous forces are dominating over the inertia forces.

2.3 Viscosity calculation

The viscosity is calculated through the total stress tensor [14], with an additional term accounting for the constraint forces on the SPH particles composing the rigid body [15].

3 APPLICATION TO SUSPENSION MODELLING

3.1 Jeffery Orbit

The rotation of particles in a shear flow is a first test of the simulation model. Jeffery’s equations describe the movement of an ellipsoidal particle in a Stokes flow [16]. This analytical model is used to analyze the results of the simulations. The rotation period with respect to shear rate and particle aspect ratio is given by:
Here $T$ is the rotation period, $r_e$ is the aspect ratio of the ellipsoids and $\dot{\gamma}$ the shear rate. $r_e = a/b$ where $a$ and $b$ are the axis of the ellipsoidal particle. The simulation setup is chosen in such a way that the simplified 2d form of Jeffery’s equations can be used:

$$T = 2\pi \frac{r_e + \frac{1}{r_e}}{\dot{\gamma}}$$

(2)

$$\phi(t) = \arctan \left( r_e \tan \frac{\dot{\gamma} t}{r_e + \frac{1}{r_e}} \right)$$

(3)

The setup consists of an ellipsoidal rigid body in a representative volume element (RVE). Through Lees-Edwards boundary conditions (LEBC) a simple shear flow (couette flow) is applied [14]. The orientation of the particle over time is compared to the analytical results of Eq. (3). Different particle shapes and resolutions were simulated. In this paper the results for one shape and three resolutions are shown, an aspect ratio of $r_e = 1.44$ is chosen as it is close to the particle shapes used in the tape casting process, investigated in [3]. Figure 1 shows the particle with the different resolutions, which, in this case, depends on the smoothing length and also the initial distance between the SPH particles. The initial distance between the particles has been set equal to the smoothing length in the following calculations.

**Figure 1:** Particle ($r_e = 1.44$) in three different resolutions (from left to right: smoothing length $h$: 0.2, 0.1 and 0.05 mm)

The length of the axis $a$ and $b$ of the particle are 1.3 mm and 0.9 mm, respectively. The edge length of the RVE is 5 mm. Viscosity of the surrounding fluid is 3 Pa s. The density was scaled to achieve bigger time steps. All following simulations are in a low Reynolds number regime were the impact of inertia is negligible compared to the viscous forces, thus the scaling of the density will not effect the outcome of the calculations.

In Fig. 2 the results of the simulations are shown as well as the analytical solution of the Jeffery orbit for the aforementioned parameters.
Not surprisingly the agreement between simulation and the analytical result is best at the highest resolution. At $h = 0.1$ mm the result is still satisfying, but at $h = 0.2$ mm the deviation is significant. The qualitative result is in accordance with the Jeffery orbit, but the quantitative result strongly depends on the resolution. However, even at the highest resolution a slight deviation is still visible, in spite of the fact that the shape of the particle is well reproduced. A likely cause for this is the RVE cell, which is small compared to the rigid body. The rotating particle causes perturbations in the flow field, which may lead to locally inhomogeneous shear rates different from the one specified on the LEBC. The shear rate around the particle in Fig. 3 shows the size and magnitude of the perturbation. Also the SPH particles inside the body behave different than normal SPH particles as they are not compressible. Furthermore the accuracy of the boundary between the particles and the fluid depends on the smoothing length (and thus also on the resolution) as SPH particles can overlap to a certain degree. So there is a difference between the volume of a rigid object composed of SPH particles and the effective volume during the simulation. This difference should be proportional to the smoothing length.

Figure 2: Orientation of the particle depending on the time at $\dot{\gamma} = 30$ 1/s and $r_e = 1.44$ (an orientation angle of 0° corresponds to a fully horizontally aligned particle)

Figure 3: Shear rate and streamlines around the particle
The result of the simulation with 0.05 mm is used to fit the shear rate in Eq. (2) to compensate the effects discussed above. This yields a shear rate of 29.51 1/s and a perfect accordance between the simulation and the analytical result is obtained. As the deviation from the nominal shear rates is small, it is conceivable that the difference is caused by the perturbation of the shear field. This would mean that at this resolution the cell size is the main cause for the deviation between simulation and analytical solution. At lower resolutions the deviation remains important, as it is not only related to the perturbation of the flow field but to the fact that the shape of the particle cannot be resolved accurately at such a coarse resolution.

3.2 Suspension viscosity

The viscosity of a suspension is determined by the viscosity of the solvent and the volume fraction of particles. In the simple case of hard spheres, taking into account the hydrodynamic interactions, the dependency is given by the Batchelor equation [17]:

$$\eta = \eta_s (1 + 2.5\phi + 6.2\phi^2)$$

(3)

where $\eta$ and $\eta_s$ are the viscosity of the suspension and the solvent, respectively. $\phi$ is the particle volume fraction. This formula is applicable to volume fractions up to $\phi < 0.1$.

Similar to the particle rotation simulations a second RVE was filled to different volume fractions with spherical rigid bodies. Here as before, it has to be taken into account that the effective volume fraction depends on the smoothing length as the SPH particles can overlap during the simulation. A correction term has been applied, taking into account the overlap and the smoothing length when generating the initial simulation setup. Table 1 contains the simulation parameters. Fig. 4 shows the initial state of the simulation with 6 % volume fraction particles.

<table>
<thead>
<tr>
<th>Table 1: Simulation parameters for the suspension viscosity simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solvent viscosity $\eta_s$</td>
</tr>
<tr>
<td>Shear rate $\dot{\gamma}$</td>
</tr>
<tr>
<td>Edge length of the RVE $d$</td>
</tr>
<tr>
<td>Particle size $d_p$</td>
</tr>
<tr>
<td>Smoothing length $h$</td>
</tr>
<tr>
<td>Volume fraction $\phi$</td>
</tr>
</tbody>
</table>
The results show a good quantitative agreement with the viscosity predicted by the theory. The comparison can be found in Fig. 5.

![Figure 4: Initial state of the RVE for the simulation with a particle volume fraction of 6 %](Image)

**Figure 4:** Initial state of the RVE for the simulation with a particle volume fraction of 6 %

![Figure 5: Viscosity in simulation and theory dependent on the particle volume fraction](Image)

**Figure 5:** Viscosity in simulation and theory dependent on the particle volume fraction

### 3.3 Anisotropy development

The rigid body model presented in this work enables the investigation of the movement of the particles inside the slurry on a microscopic scale. The focus is on the orientation of the particles in a shear flow with a volume fraction as typically used for tape casting and different particle aspect ratio. The purpose of these simulations is to investigate the limits of applicability of Jeffery’s equation at higher volume fractions. To compare the results the analytical Jeffery’s equation was solved numerically for a system with a high number of initially randomly orientated particles with different shapes. Thus, it should be possible to see the effects of the hydrodynamic interactions and particle collision on the orientation of the particles as these are not taken into account in Jeffery’s equation.

The simulation setup is identical to those in section 3.2. The main differences are the larger RVE to particle size ratio and the use of non-spherical particles. Three particle aspect ratios were used. All parameters were chosen in the range typically used in tape casting. The parameters can be found in Table 2.
Table 2: Simulation parameters for the orientation simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solvent viscosity $\eta_s$</td>
<td>0.42 Pa s</td>
</tr>
<tr>
<td>Shear rate $\dot{\gamma}$</td>
<td>60 1/s</td>
</tr>
<tr>
<td>Particle size $d$</td>
<td>35 $\mu$m</td>
</tr>
<tr>
<td>Smoothing length $h$</td>
<td>4 $\mu$m</td>
</tr>
<tr>
<td>Volume fraction $\phi$</td>
<td>22 %</td>
</tr>
<tr>
<td>Aspect ratio $r_e$</td>
<td>1.0, 1.25, 1.5</td>
</tr>
</tbody>
</table>

Fig. 6 shows the results of the simulations. Periodic oscillations are visible on the solid line showing the momentary average orientation. As the systems consist of about 180 particles the curve is not smooth as the amount of particles is not sufficient to get satisfying statistics. The dashed line is the running average, which can be used to compare the results of the simulation with the analytical calculation. In Table 3 the results for both are shown. As the differences between the analytical calculation and simulation are small, it is reasonable to assume that the particles are not significantly disturbed by interaction with other particles in their rotation, at least for the volume fraction and particle shapes studied here. At higher aspect ratio the difference becomes higher, one explanation for this behaviour is that the more elongated the particles are the higher the chance that they hinder each other in their rotation. This might not be applicable to particles with even higher aspect ratios then those studied in this work, as other effects might influence the particle orientation in these areas. To make a more general statement concerning the behaviour of particulate suspensions, the system has to be investigated in more detail over a broader range of particle shapes and volume fractions.

Figure 6: Average (solid line) and running average (dashed line) orientation of the particles depending on the aspect ratio (an orientation angle of $45^\circ$ corresponds to a system with a random particle orientation, lower angles to a horizontal alignment and higher angles to vertical alignment)
Table 3: Comparison between numerically and analytically calculated average particle orientation

<table>
<thead>
<tr>
<th>r_e</th>
<th>( \phi_{\text{theory}} )</th>
<th>( \phi_{\text{sim}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>45.00°</td>
<td>45.69°</td>
</tr>
<tr>
<td>1.25</td>
<td>49.10°</td>
<td>50.08°</td>
</tr>
<tr>
<td>1.5</td>
<td>52.24°</td>
<td>54.41°</td>
</tr>
</tbody>
</table>

4 SUMMARY AND OUTLOOK

An SPH simulation model with solid-fluid coupling for suspensions with non-spherical particles has been developed. Different verification tests have been made, which show a good agreement with theoretical predictions. The model was then used to investigate the influence of the particle shape on the orientation of particles in flow conditions which are typical for tape casting. It has been shown that the orientation in the green tape is linked to the rotation of the particles in the shear field under the blade. The orientation of the particles depends on the particle shape and the volume fraction. The analytical Jeffery’s equation for the rotation of the particles seems to give a good estimate for the particle alignment at least for volume fractions below 25% and small particle aspect ratios. At the highest particle ratio used in this work the Jeffery’s equation underestimates the orientation.

In future, the model will be enhanced to be able to simulate more complex suspensions. In realistic suspension the short range van der Waals forces, which draw the particles together, are counteracted by electrostatic or steric forces which stabilize the suspension. Also more precise contact forces, as those typically used in DEM simulation, will be implemented to describe the collisions between rigid bodies more thoroughly. This should also enable an even more detailed modeling of the slurries used in tape casting.

5 ACKNOWLEDGEMENT

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REFERENCES


MOLECULAR-DYNAMICS INVESTIGATION OF NANO-BURNISHING PROCESS

VIKTOR P. KUZNETSOV‡, ANTON Y. NIKONOV*† AND ANDREY I. DMITRIEV*†

‡ Kurgan State University (KgSU)
25, st. Gogolya, 640000, Kurgan, Russia
email: wpkuzn@mail.ru - Web page: http://www.kgsu.ru

* Institute of Strength Physics and Materials Science SB RAS (ISPMS SB RAS)
2/4, pr. Akademicheski, 634021 Tomsk, Russia
e-mail: dmitr@ispms.tsc.ru, www.ispms.ru

† Tomsk State University (TSU)
36, pr. Lenin 634050 Tomsk, Russia

Key words: Molecular Dynamics, Contact Problems, Burnishing, Nano-fragmentation.

Abstract. It is well known that the burnishing process affects the surface characteristic, namely: surface roughness, surface hardness, wear resistance, fatigue resistance and increased maximum residual stress in compression. Unfortunately we still far from full understanding what parameters and mechanisms are responsible for the certain surface modification. That is why methods of computer modeling can be considered as useful tool to investigate surface changing during contact interaction as well as burnishing process. It is more essential if we consider processes are taking place at atomic scale level.
In the paper we try to reproduce the details of burnishing process at nano-scale level. To investigate features of surface treatment we use the molecular dynamics simulation. Various pure crystalline materials were considered. Results of our modeling are very close to the experimental observation

1 INTRODUCTION

Performance of various assemblies and machine components are determined by the qualitative characteristics of the surface layer, resulting during the finishing treatment. One of the modern techniques of high surface finish of parts in mechanical engineering is a method of surface plastic deformation, which is called as burnishing. It was established that the burnishing improves wear resistance of parts by 20-40%, fatigue by 30-70%, resistance to contact fatigue by 20-40% [1]. Changing the properties of surfaces after burnishing is connected with the change in the structure of a thin surface layer due to plastic deformation. Under the influence of the indenter motion change of orientation and shape of grains, which are crushing, flattening and stretching, forming the texture of the surface layer [2] are taken place.

It is extremely difficult to investigate the structural changes occurring in the surface layer of material directly during the burnishing. In this regard, methods of computer simulation can
be an important complement to experimental studies. However, models based on the methods of continuum mechanics do not allow us to reveal the mechanisms of structural rearrangements in the surface layer of the material. Therefore, the purpose of this research was to study the origination and development of structural defects by modeling of nanoburnishing with help of molecular dynamics method [3, 4].

2 DESCRIPTION OF THE SETUP

A copper crystallite was chosen as a model material to investigate the result of nanoburning process. The interatomic interaction was constructed within the embedded-atom method [4, 5]. This potential with a high accuracy describes the elastic and surface properties as well as energy parameters of the defects of the modeled system. The equations of motion were integrated with time step \( \Delta t = 0.001 \) ps. The calculations were performed on a multiprocessor cluster «Skif Cyberia» using a software package LAMMPS [6]. The total number of atoms exceeds 1.5 million. The simulated crystal was oriented in such a way that the crystallographic directions [100] [010] and [001] of fcc lattice were corresponded to the X, Y and Z axis. Dimensions of the model sample in the direction of the coordinate axes were equal to 40.13 x 24.95 x 16.63 nm, respectively.

The scheme of the model sample is shown in Figure 1. The roughness of the surface layer with a maximum depth of 2.5 nm was specified directly in the simulated crystallite at the initial stage. The roughness was created by the removal of surface-layer atoms that fall within the sphere of radius, which ranged from 0 to 2.5 nm. Center of the sphere was located at the level of the surface layer, and its position in the plane XoZ was determined using random numbers. The periodic boundary conditions were simulated in the Z direction. Thus the replication of the simulated fragment allows one to simulate the length of the sample in a given direction. Surfaces along X and Y axis were simulated as free. The lower layer of atoms (dark bottom layer in Figure 1) was fixed, imitating the unmovable substrate. Thickness of the substrate was 0.73 nm. Over the substrate a special "damping" layer of atoms, which used the procedure to reduce the kinetic energy accumulated due to dynamic loading was added. Introducing of such layer with properties of heat transfer allows us to take into account the length of the sample depth of the material in Y direction. The thickness of the "damping" layer was 1.45 nm. Its kinetic temperature - the temperature obtained from the equality of thermal and kinetic energy, was maintained in the range from 125K do135K.

![Figure 1: The scheme of the modeled sample](image)
The burnishing was performed using an indenter, whose action has been realized through the force field in the shape of the cylinder with the axis along the axis Z and a certain radius. On the atoms that fall into this area, forces acting in the direction from the axis of the cylinder. The direction and magnitude of the force is described by \( F(r) = -K(r - R)^2 \) where \( K \) - constant, \( r \) - distance from the center of the cylinder to the atom, and \( R \) - radius of the cylinder, while at \( r > R \) \( F(r) = 0 \). The burnishing of the model sample was carried out using two indenters with radii differ by 4 times: 4 nm and 16 nm.

3 RESULTS OF MODELING

3.1 Burnishing using the indenter with a radius of 4 nm

Results of simulation showed that the nano-burnishing by cylindrical indenter with radius of 4 nm on a small spatial interval resembles the process of cutting or scratching. When the indenter moves horizontally a "bead" forms before it from the atoms of the upper layer. As it moves, the height of "bead" is growing. This is clearly seen in Fig. 2, which shows the topography at different times of a single central layer of atoms arranged in parallel planes XoY. Arrow indicates the position of the axis of the cylindrical indenter at a given time. If we compare the surface profile before and after the passing of the indenter (for example, in Fig. 2 profiles at \( t = 0 \) and \( t = 2 \) ns), we can see that the characteristic size of the roughness of the surface layer decrease markedly. The difference in the scale reaches one order as for given sizes of the modeled object may be interpreted as a modeling of burnishing. Indeed, after the passage of the indenter the surface roughness does not disappear completely, but it is decreasing. Indenter geometry (small size or large curvature radius) leads to generation of a "bead" in front of its motion from the atoms of the surface layer. This should further increase the resistance force of the indenter movement. We should expect that at a certain magnitude of the resistance force the indenter starts to move in the Y direction over the surface of the crystallite, thereby creating an induced periodic roughness due to the peculiarities of the process. Such behavior can be compared with the results of nano-burnishing within the dynamic instability of the process.

Figure 3 shows the structure of the simulated crystallite at time \( t = 2 \) ns. The position of surface atoms along the axis Y is marked by color: from blue to red. The layer which location corresponds to a penetration depth of the indenter (\( y = -3 \) nm) is selected as a basic level.

To analyze the peculiarities of structural transformations during the nano-burnishing process the special algorithm to search the local structural changes was used. This algorithm allows one to identify the generation of defects such as dislocations and stacking faults in the fcc lattice. Description of the algorithm is given in [7]. According to the results during the treatment of the modeled sample there are numerous structural defects are nucleated in the bulk of the material. Movement of the indenter leads to growing of its number, and they extend from the surface into the bulk material. Thus, as a result of plastic deformation formed a modified surface layer with properties different from properties of the material in bulk. Formation of numerous defects in the surface layer also means the possibility to form nano-fragment structure with misoriented nano-grains.
Figure 2: The surface profile of the modeled crystallite at different times. By arrow the position of center of the indenter is shown. At time t=0 the indenter was located over the surface of the crystallite.

Figure 3: The structure of the modeled crystallite at time t=2 ns.

Figure 4 shows the simulated fragment at the time when the structure of surface defects was formed. Centers of the atoms with a local topology of the structural bonds of the fcc lattice, marked with small dots (non-defected areas). Centers of the atoms with a local topology of the structural links which is different from the fcc lattice are marked by large dots. For better visualization centers of surface atoms are marked by small red dots.

Figure 4: 3D visualization of local structure transformations in the modeled crystallite at time t=1.8ns.
3.1 Burnishing using the indenter with a radius of 16 nm

Due to the size of the indenter with a radius of 16 nm were comparable to the size of the modeled crystallite, the algorithm of loading to imitate the burnishing process was differed from the previous case. Thus, the initial position of the center of the indenter was set outside of the modeled fragment. Then, as in the first case, the load was specified in two stages: indentation and phase of horizontal movement of the indenter. As a result of indentation the left edge of the modeled fragment was exposed to the forces from the force field of the indenter, which, as in the previous case, was pressed into a depth of 3 nm, comparable to the maximum surface roughness.

After reaching a certain depth of the indenter penetration a relaxation stage during 5 ps was modeled. In the second stage of loading the motion of the indenter alone X-axis (Fig. 5) with a constant velocity 10 m / sec was simulated. During all calculation the indenter moves along the X axis on the distance of 56nm.

According to the results of calculation treatment of the modeled crystallite with bigger indenter as a process closer to the real technological burnishing, because of small curvature of the indenter less contributes to a "bead" formation of the atoms of the surface layer. The indentation of individual rough surface in the volume of material that gives rise to both plastic and a large part of the elastic components of deformation in surface layer. In the central part of the modeled fragment smoothing of initial roughness of the surface layer within one order of magnitude (from 2 nm to 0.5 nm) is taking place. However, a significant part of stored elastic strain conditional by small curvature of the indenter, leads to the fact that during unloading (after passing of the indenter), the level of the surface restore by an average of 0.5 nm to a value of \( y = 22.5 \text{nm} \) (Fig. 6).

Fig. 7 shows the structure of the model crystal at time \( t = 4\text{ns} \). The position of surface atoms along the axis Y is marked by color: from blue to red. The layer which location corresponds to a penetration depth of the indenter (\( y = -3 \text{nm} \)) is selected as a basic level.

Analysis of structure of the modeled crystallite showed that larger number of different structural defects appears bulk in the sample than in case of the indenter with a radius of 4 nm. This difference is due to the greater area of contact and a greater degree of deformation.
Figure 6: The surface profile of the modeled crystallite at different times. By arrow the position of center of the indenter is shown. At time $t=0$ the indenter was located on the left and over the surface of the crystallite.

Figure 7: The structure of the modeled crystallite at time $t=4$ ns By color the vertical position of surface atoms is indicated.

Figure 8: 3D visualization of local structure transformations in the modeled crystallite at time $t=3.5$ ns.
During the tangential motion of the indenter number of structural defects is also growing, and they extend from the surface into the bulk material. Thus the result of plastic deformation is the formation of a modified surface layer with properties different from properties of the material in bulk. Analyzing the structure formed by many intersecting planes of stacking faults it is possible to say about generation of nano-fragmentation structure in the surface layer of the modeled fragment. Figure 8 shows the simulated fragment at time when the structure of surface defects was formed. Centers of the atoms with a local topology of the structural bonds of the fcc lattice, marked with small dots (non-defected areas). Centers of the atoms with a local topology of the structural links which is different from the fcc lattice are marked by large dots. For better visualization centers of surface atoms are marked by small red dots.

4 CONCLUSIONS

In conclusion, we note that the results of computer simulations agree well with experimental data, obtained using scanning electron microscope Tescan Mira 3 LMU [8]. So, fig. 9 shows the structure of the surface layer of steel 20X13 at the initial state and subjected to burnishing processing of diamond spherical indenter with a radius of sharpening R = 4 mm. Applied force P = 230 N, feed S = 0,08 mm / rev, speed burnishing V = 100 m / min. It was established that nano-burnishing leads to structure changing in a thin surface layer, namely, as a result of plastic deformation is the formation of fine-grained structure, which increases the microhardness, elastic limit and yield strength of the surface layer [1].

**Figure 9:** Structure of surface layer of steel 20X13: a) initial state and b) after nano-burnishing with diamond indenter.
REFERENCES


SOFT VERSUS HARD METASTABLE CONFORMATIONS IN MOLECULAR SIMULATIONS

Konstantin Fackeldey*, Susanna Röblitz*, Olga Scharkoi* AND Marcus Weber*

*Zuse Institute Berlin (ZIB)
Takustrasse 7
14195 Berlin, Germany
e-mail: {fackeldey, susanna.roeblitz, scharkoi, weber}@zib.de, www.zib.de

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Abstract. Particle methods have become indispensable in conformation dynamics to compute transition rates in protein folding, binding processes and molecular design, to mention a few. Conformation dynamics requires at a decomposition of a molecule’s position space into metastable conformations. In this paper, we show how this decomposition can be obtained via the design of either “soft” or “hard” molecular conformations. We show, that the soft approach results in a larger metastability of the decomposition and is thus more advantageous. This is illustrated by a simulation of Alanine Dipeptide.

1 Introduction

In practice, molecular simulations are carried out by solving the equations of motion of molecular dynamics. The solution of the ordinary differential equation results in a trajectory in state space (position and momentum space) and is a model for a closed system behavior of the molecule, i.e. a simulation at constant energy. The trajectory is analyzed in position space in order to derive statistical information about the molecular system. In this article, we focus on simulations at constant temperature (canonical ensemble) instead of constant energy (microcanonical ensemble). The dynamical system under consideration is a Markov chain in position space which will be derived in the next section.

Molecular simulations are not as easy as it seems at a first glance. If we observe certain internal coordinates of a simple molecule (like the C-C-C-C torsion angle of butane in Figure 1), we see that the mentioned Markov chain comprises metastabilities. The system jumps between so-called metastable conformations. The aim of conformation dynamics is to analyze this jump process, i.e. to identify the metastable conformations in position space, their statistical weights, and to compute the transition probabilities between them [1, 2, 9].
Although it seems to be a good idea to derive this information from a long-term Markov chain, the metastabilities are problematic from a statistical point of view. Since jumps between metastable conformations are rare events, even a long-term simulation (carried out by the largest parallel computing machines) does not provide enough statistical information for the derivation of the transition patterns. Furthermore, counting the number of Markov states per metastable conformation is not a good idea for deriving statistical weights of the conformations, because rapid (global) equilibration is avoided by the rare events.

A rather old idea to circumvent the problem of simulation in the presence of high-energy barriers is given by transition state theory. In this context, many researchers think of a one dimensional reaction coordinate (plotting the reaction coordinate against the free energy level). Two minima representing the educt as well as the product, respectively. An energy barrier between these two states has a local maximum (the transition state). Furthermore, the energy difference between the transition state and the minimum determines the reaction rate.

This simple picture does not hold for all kinds of molecular simulations. Briefly, the higher the barrier the better are the results from transition state theory. In conformation dynamics this insufficient picture is corrected. The metastable conformations are not defined as local minima of a free energy landscape. In contrast, the whole high-dimensional position space is decomposed into metastable conformations. More precisely, in Figure 1 the y-axis (representing the position space) may be decomposed into three intervals which are called metastable conformations in this context. Transition state theory searches for a certain point at which the molecular system switches from conformation A to conformation B, whereas a conventional, set-based decomposition approach of conformation dynamics aims at finding high-dimensional transition "hyper planes". In this article, we will replace these transition hyper planes by soft barriers. That means we will replace a set-based decomposition of the position space (hard clustering) by a partition of unity decomposition of the position space using membership functions (soft clustering). Although it seems that this soft clustering leads to rather "unstable" metastable conformations, this is not true. We will give an illustrative example in section 5. In fact, our approach provides conformations with the highest "metastability" and (assuming a perfect discretization) the systematic error of the set-based transition rates described by [8] vanishes. Simply speaking, our more complex picture does hold for all molecular systems and provides an effective analysis of the transition pattern between molecular conformations.

2 Statistical Mechanics

In a canonical ensemble the state of a biomolecule is not described by a single global minimum energy structure, but by a statistical ensemble in a phase space $\Gamma$. For $x = (q, p) \in \Gamma = \Omega \times \mathbb{R}^d$ the positions $q$ and momenta $p$ of each atom in the molecule are given
Figure 1: The longterm simulation of butene clearly shows three metastable conformations of the molecule.

according to the Boltzmann distribution:

\[ \pi(q, p) \propto \exp(-\beta H(q, p)). \] (1)

Here \( \beta = 1/k_B T \) is the inverse temperature \( T \) multiplied with the Boltzmann constant \( k_B \), and \( H \) denotes the Hamiltonian function which is given by \( H(q, p) = V(q) + K(p) \), where \( V(q) \) is the potential and \( K(p) \) the kinetic energy. This canonical density can be split into a distribution of momenta \( \eta(p) \) and positions \( \pi(q) \) where

\[ \pi(q) \propto \exp(-\beta V(q)) \] and \( \eta(p) \propto \exp(-\beta K(p)) \).

Let us consider the Hamiltonian dynamics which is given by

\[ \dot{q} = p, \quad \dot{p} = -\nabla V(q), \] (2)

where \( \nabla V(q) \) is the gradient of an energy function (the potential) \( V : \Omega \to \mathbb{R} \). It is well known, that (2) can be the starting point for a trajectory based description of this system in a microcanonical ensemble. In contrast, we now consider a system which is embedded in a heat bath with constant temperature \( T \) in a canonical ensemble. According to (2) the corresponding flow \( \Phi^\tau \) for a time span \( \tau > 0 \) is given by

\[ (q(t), p(t)) = \Phi^\tau(q_n, p_n), \quad n \in \mathbb{N}. \]

Let \( \Pi_q \) be the projection of the state \( (q, p) \) onto the position \( q \) and let further \( p \) be chosen randomly according to the distribution \( \eta(p) \), then

\[ q_{i+1} = \Pi_q \Phi^\tau(q_i, p_i) \]
describes a Markov process. The $i$th state depends on the preceding state only.

It can be shown, that this assumption of Markovianity implies that the corresponding Liouville operator is time independent e.g. [9]. By projecting this Liouville operator onto the position space the behavior of the system can be described by a transition function [9], which is given by

$$p(\tau, f, h) = \int_{\Omega} T^\tau f(q) h(q) \pi(q) dq,$$

(3)

where

$$T^\tau f(q) = \int_{\mathbb{R}^d} f(\Pi_q \Phi^\tau(q, p)) \eta(p) dp.$$  

(4)

This construction offers many advantages for the analysis of molecular processes. The fundamental idea behind this formulation is, that the transfer operator $T^\tau$ in (4) is a linear operator although the ordinary differential equation (2) is (extremely) non-linear. This linearization allows for a Galerkin discretization of $T^\tau$ and thus for a numerical approximation of eigenfunctions and eigenvalues of the discrete spectrum of $T^\tau$.

We take advantage of the fact, that the behavior of molecules can be well described by its structurally related configurations (metastable conformations). Mathematically speaking, a metastable conformation is a function $C: \Omega \rightarrow [0, 1]$ which is nearly invariant under the transfer operator $T^\tau$, i.e.

$$T^\tau C(q) \approx C(q).$$

In the following we show how the metastable conformations can be computed via a discretization of the position space.

3 Discretization

In order to “resolve” or to identify the metastabilities we need a discretization of the position space. At this stage, we define a decomposition of $\Omega$, which we need in order to employ our techniques. Let therefore $\{\theta_i\}_{i=1}^N$ be a set of basis function and $\Omega_i = \text{supp}(\theta_i) \forall i = 1, ..., N$. We say that the basis functions $\{\theta_i\}_{i=1}^N$ are a hard decomposition of $\Omega$, if
i) $\Omega_i$ is measurable and $|\Omega_i| > 0$ for $i = 1, \ldots, N$

ii) $|\Omega_i \cap \Omega_j| = 0$ if $i \neq j$

iii) $\sum_{i=1}^{N} \theta_i(q) = 1$, $q \in \Omega$.  

As we have already mentioned, the position space is high dimensional which prohibits any usage of meshbased methods like finite elements. Thus we take advantage of meshfree methods, more precisely we consider a Voronoi tessellation. We choose characteristic basis functions $\{\chi_i\}_{i=1}^{N}$ with $\chi_i : \Omega \rightarrow \{0, 1\}$ defined by

$$
\chi_i(q) = 1_{\Omega_i}(q) := \begin{cases} 
1 & \text{if } q \in \Omega_i \\
0 & \text{otherwise}
\end{cases}
$$

Obviously, these basis functions suit the requirements of a hard decomposition. Moreover it is easy to see that the $\chi_1, \ldots, \chi_N$ form a partition of unity, i.e.

$$
\sum_{i=1}^{N} \chi_i(q) = 1 \quad \text{and} \quad \chi_i \geq 0 \quad \forall i.
$$

In terms of the characteristic basis functions $p(\tau, \chi_i(q), \chi_j(q))$ describes the transition probability between the two sets $\Omega_i$ and $\Omega_j$. In other words, it describes the ratio of trajectories starting in $q \in \Omega_i$ with Boltzmann distributed momenta $p \in \mathbb{R}^d$ and ending in $\Omega_j$ after timespan $\tau > 0$.

Having now a discretization of $\Omega$ we can give the metastabilities a more precise meaning. To do so, we aim at a set $\{C_1, \ldots, C_{n_c}\}$ such that $\sum_{J=1}^{n_c} C_J(q) = 1_{\Omega}$ $\forall q \in \Omega$ where $C_J : \Omega \rightarrow [0, 1]$ is a function. Then we can define each $C_J$ as a linear combination of the basis functions $\{\chi_i\}_{i=1}^{N}$. More precisely

$$
C_J(q) = \sum_{i=1}^{N} G_{iJ} \chi_i(q), \quad J = 1, \ldots, n_c. \tag{6}
$$

Here and in the forthcoming, we use capital $I, J, \ldots$ indices for numbering of the metastable conformations. In order to employ a Galerkin discretization, we define $\langle g, f \rangle_\pi = \int_{\Omega} f(q)g(q)\pi(q)\,dq$ and insert (6) into (5), s.th.

$$
\langle T^\tau \sum_{i=1}^{N} G_{iJ} \chi_i \rangle_\pi \approx \sum_{i=1}^{N} \langle G_{iJ} \chi_i, \chi_j \rangle_\pi
$$

$$
\sum_{i=1}^{N} \langle T^\tau G_{iJ} \chi_i, \chi_j \rangle_\pi \approx \sum_{i=1}^{N} \langle G_{iJ} \chi_i, \chi_j \rangle_\pi. \tag{7}
$$
Since \( \langle \chi_i, \chi_j \rangle_\pi = \delta_{ij} \langle \chi_j, \chi_j \rangle_\pi \) we obtain

\[
\sum_{i=1}^N G_{ij} \langle \chi_i, \chi_j \rangle_\pi = G_{jj} \langle \chi_j, \chi_j \rangle_\pi.
\]

Thus (7) is equivalent to

\[
\sum_{i=1}^N G_{ij} \langle T^\tau \chi_i, \chi_j \rangle_\pi \approx G_{jj} \langle \chi_j, \chi_j \rangle_\pi.
\] (8)

Dividing both sides of (8) by \( \langle \chi_j, \chi_j \rangle_\pi \) we can define

\[
P_{ji} = \frac{\langle \chi_j, T^\tau \chi_i \rangle_\pi}{\langle \chi_j, \chi_j \rangle_\pi} = \int_{\Omega} T^\tau \chi_i(q) \frac{\chi_j(q)}{\int_{\Omega} \chi_j(q) \pi(q) dq} dq
\]

and we obtain for the coefficients \( G_{ij} \)

\[
P^\tau g_j \approx g_j,
\] (9)

where \( g_j = [G_{1j}, G_{2j}, \ldots, G_{Nj}]^T \). The stochastic matrix \( P^\tau \) describes the transition probabilities between the basis functions.

We remark that the computation of the above integral is a challenging task, since the underlying space is high dimensional. To overcome this, we employ strategies from particle methods. In detail, we apply Markov chain Monte Carlo methods [4] in each Voronoi cell to generate a local Boltzmann distribution \( \pi_i(q) \) for each of the basis functions \( \{\chi_i\}_{i=1}^N \), i.e.

\[
\pi_i(q) = \frac{\chi_i(q)}{\int_{\Omega} \chi_i(q) \pi(q) dq}.
\]

The sampled positions \( q \) are propagated by molecular dynamics according to \( \Phi^\tau \) with randomized initial momenta. With these data we compute the entries of \( P^\tau \). So far we have not given any details for the matrix \( G \) in (6). Let us therefore point out the two following aspects:

- The coefficients \( G_{ij} \) can then be computed as a linear combination

\[
G = X A
\]

of the eigenvectors \( X \) of \( P^\tau \) corresponding to eigenvalues close to one. For the \( n_c \) metastable conformations, \( T^\tau \) has a cluster of eigenvalues \( \lambda_i \) close to one, i.e. \( 1 = \lambda_1 > \lambda_2 > \ldots > \lambda_{n_c} = 1 - \epsilon \gg \lambda_{n_c+1} \ldots \) [9]. Therefore, single eigenvectors are ill-conditioned, whereas the invariant subspace \( \mathcal{X} = \text{span}(g_1, \ldots, g_{n_c}) \) is well conditioned. The matrix \( A \in \mathbb{R}^{n_c \times n_c} \) is some unknown non-singular transformation matrix. Every matrix \( G \) obtained by such a transformation of eigenvectors satisfies the invariance condition (9).

Among all possible transformation matrices \( A \), we would like to find one that results in vectors \( g_j \) with special properties.
The matrix $G$ plays an important role, since each entry $g_{iJ}$ of $G$ relates the basis function $\chi_i$ to the metastable conformation $C_J$. In the original work [2], the conformations $\{C_1, ..., C_{n_c}\}$ are built as hard decomposition, such that the matrix $G$ has only the entries 0 and 1. However correspondingly, to the definition of the hard decomposition, we can also define a decomposition soft if it meets the same conditions as a hard decomposition except for the fact, that

ii*) $|\Omega_i \cap \Omega_j| \geq 0$ if $i \neq j$,

i.e. we allow an overlap of the $\Omega_i$.

As a consequence the entries in the matrix $G$ can take all values between 0 and 1 [3]. This allows us to assign for each basis function $\chi_i$ a certain degree of membership to each conformation. In other words, the $i$th row of $G$ shows how much the $i$th basis function “contributes” to each metastability. In Figure 3 the difference between the soft and hard decomposition is shown.

Since every soft clustering can always be relaxed to a hard one, our goal is to find a soft partitioning of the position space. Thus, we have to find a non-singular transformation matrix $A$ such that $G$ describes a soft partitioning. The computational details will be explained in the following section.

### 4 Clustering

The conditions on $G$ discussed in the previous section can be summarized as follows:

(i) $G_{iJ} \geq 0 \quad \forall i \in \{1, \ldots, N\}, \ J \in \{1, \ldots, n_c\}$  \hspace{1cm} \text{(positivity)}

(ii) $\sum_{J=1}^{n_c} G_{iJ} = 1 \quad \forall i \in \{1, \ldots, N\}$  \hspace{1cm} \text{(partition of unity)}

(iii) $G = XA$ where $P^T X = X\Lambda$, $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_{n_c})$, $A$ non-singular  \hspace{1cm} \text{(invariance)}

Among the feasible transformation matrices we seek for a matrix $A$ such that the resulting membership vectors $g_J$ are as characteristic as possible ($|\Omega_i \cap \Omega_j| \approx 0$).
This can be achieved by maximizing the objective function

\[
I(\mathcal{A}; X, \pi) = \frac{1}{n_c} \sum_{i=1}^{n_c} \frac{(\chi_i, \chi_i/\pi)}{(\chi_i, e)_\pi} \leq 1, \tag{10}
\]

where \( e \) denotes the vector with all entries equal to 1. One has to maximize a convex function with linear constraints. The optimization problem can be solved by the Nelder-Mead algorithm provided that a good initial guess for \( \mathcal{A} \) is available. This starting guess is obtained by the inner simplex algorithm as described in [10]. The maximization of (10) subject to the constraints (i) to (iii) is called Robust Perron Cluster Analysis (PCCA+) [3, 7].

Once the membership vectors \( g_J \) have been computed, one can compute a coarse grained transition probability matrix \( P_c \) by projecting the original matrix \( P^\tau \) onto the metastable conformations,

\[
P_c = (G^T w_D G)^{-1} G^T w_D P^\tau G, \tag{11}
\]

where \( w_D \) denotes a diagonal matrix with the stationary distribution \( w \) of \( P \) \( (w^T P^\tau = w^T) \) on the diagonal. The matrix \( P_c \) is not necessarily a stochastic matrix because it can have negative entries if the membership vector \( g_J \) are far from being characteristic. However, \( P_c \) has row sum one and is the correct propagator for densities restricted to the metastable conformations [6]. In fact, \( \det(P_c) \) is a measurement for the metastability of the decomposition defined by \( G \) [11]. It holds

\[
P_c = \mathcal{A}^{-1} \Lambda \mathcal{A}, \quad \text{thus } \det(P_c) = \prod_{i=1}^{n_c} \lambda_i.
\]

It has been shown that for any \( G \) satisfying (i) and (ii), \( \det(P_c) \) can be bounded from above by \( \prod_{i=1}^{n_c} \lambda_i \) [11]. Thus condition (iii) ensures a decomposition with maximal metastability.

Since the number of clusters \( n_c \) is unknown in advance, it is recommended to run the cluster algorithm several times with different input values for \( n_c \) and to choose the “best” solution for which \( I(\mathcal{A}; X, \pi) \) is maximal.

### 5 Example

We demonstrate the application of our algorithm to the model system alanine dipeptide in vacuum with the mmff forcefield [5], Figure 4. For the discretization, we chose \( N = 504 \) molecular configurations from a high temperature (1000 Kelvin) molecular dynamics trajectory as defining nodes of our Voronoi basis functions \( \{\chi_i\}_{i=1}^N \). As distance measure, we use the Euclidean distance in the space spanned by the four backbone torsion angles \( \omega_1, \ldots, \omega_4 \). We thus ignore variability in other degrees of freedom, which is justified by the fact that the torsion angles are the slow degrees of freedom and that is what we are interested in. Within every basis function, a Markov chain Monte Carlo method
Figure 4: Left: Spatial structure of alanin dipeptid. Right: Chemical structure of alanin dipeptide.

Figure 5: Left: Image of the $504 \times 504$ transition probability matrix $P$ (for ease of visualization, we plotted the element-wise logarithm $\log(P)$ instead of $P$). Right: The first 10 eigenvalues of $P$. The first 5 eigenvalues form a cluster that is clearly separated from the rest of the spectrum.

Figure 6: Left: The value of the objective function (10) for different numbers of clusters. The maximum value is achieved for $n_c = 5$ clusters. Right: Image of $\log(P)$ with rows and columns resorted according to the decomposition into 5 clusters.
was applied to generate configurations distributed according to the partial densities $\pi_i(q)$. These configurations were propagated according to the flow $\Phi^\tau$ with $\tau = 39$ femtoseconds. With these data we computed the entries of the transition probability matrix $P^\tau$, which are visualized in Fig. 5. $P^\tau$ has a cluster of 5 eigenvalues close to one, and the value of the objective function (10) is also maximal for $n_c = 5$. Thus we computed the membership matrix $G$ for $n_c = 5$ clusters. The metastability of this decomposition amounts to $\det(P_c) = 0.342$. For comparison, we calculated the relaxation of $G$ towards a hard decomposition $\tilde{G}$, i.e.

$$\tilde{G}_{iJ} = \begin{cases} 1, & \text{if } J = \arg \max_j G_{ij} \\ 0, & \text{else} \end{cases}$$

The metastability of the hard decomposition amounts to only 0.264. This hard decomposition, however, can be used to visualize the metastable conformations. Fig. 7 shows the nodes of the basis functions colored according to the final decomposition.

### 6 Conclusions

Starting from a discretization of the position space $\Omega$ we employed two different ways to describe the metastable configurations as a linear combination of eigenvectors. In the first method we took coefficients 0 or 1, and named these metastable conformations hard. In the second method we used soft metastable conformations by allowing the coefficients to take values between 0 and 1. We have employed an example molecule and compared the performance of the soft versus hard metastable conformations. In good agreement with our theory, the soft decomposition leads to a larger metastability than the hard decomposition.
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ON THE GPU COMPUTING OF MASSIVE FORMING PROCESS SIMULATIONS

G.-P. Ostermeyer, K. Fischer
Institute of Dynamics and Vibrations (IDS)
Technische Universität Braunschweig
Schleinitzstr. 20, 38106 Braunschweig, Germany
e-mail: gp.ostermeyer@tu-braunschweig.de, ka.fischer@tu-braunschweig.de, www.ids.tu-bs.de

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Abstract. This contribution presents a modelling tool for massive forming processes that is based on a particle method. The introduced model is able to represent the realistic behaviour of different types of forming processes. As these systems usually require large amounts of particles, the potential of GPU Computing with CUDA as a possibility for performance enhancement of particle simulations is analyzed as well.

1 INTRODUCTION

The Finite Element Method (FEM) is the common tool to model massive forming processes. This method is able to deliver all the necessary information (cf. figure 1) in order to develop and optimize massive forming processes. Among these are the information e.g. on workpiece’s structural defects, on the mould filling behaviour (whether or not a mould could be completely filled under the given circumstances), on the microstructural transformation that is directly correlated to the natural stain, on the material flow and the flow lines or on the stress and temperature distribution throughout the workpieces and tools.

Although delivering quite realistic simulation results in many cases, FEM is not able to reproduce all the upcoming phenomena like mould filling errors or workpiece’s structural defects. The reason for this lies in the fact, that a correct macroscopic description of friction and wear during the forming process has not been derived yet [1]. Therefore the idea of modelling massive forming processes with particle methods is motivated, because particle methods do not depend on those macroscopic laws [2].

Despite the problem of mould filling errors, large deformations, flashing or the generation of wear require frequent remeshing during a FEM simulation. This results in a considerable increase of computational effort and therewith worsens the overall performance. The computational effort of particle simulations instead is in principal independent of the type and degree of deformation like flashing or generation of wear.
2 MESOSCOPIC PARTICLE METHOD

The particle method used in order to model massive forming processes is the mesoscopic particle method introduced in [3, 4] where the particles have additional hidden degrees of freedom. In general, for the given application, the system is discretized by rigid particles. The system’s particles interact with each other via local and predefined interaction laws. These laws have to be chosen in such a way, that a realistic macroscopic material behaviour is represented. There are different approaches to derive them. One possible way is the explicit implementation of a macroscopic stress strain relationship. Another approach considers interaction potentials similar to those used in molecular dynamics like the Lennard-Jones potential. In either case, the discretization results in a usually large amount of additional degrees of freedom, that are of course not visible from the macroscopic point of view. Thus, they are also called submechanical or hidden degrees of freedom.

In order to generate the macroscopic system performance, the information have to be transferred form the chosen discretization scale with its hidden degrees of freedom to the macroscale. Considering forming processes, especially the information on the macroscopic temperature distribution -as a result of heat generation during the forming process- is of utmost importance.

On the atomic scale, molecular dynamics use statistics in order to model the macroscopic heat generation and temperature distribution correctly. But in contrast to the atomic scale, macroscopic properties like temperature can directly be assigned to the particles. Therefore, in order to take into account the mechanical as well as the thermodynamical degrees of freedom, viscous dampers are used to separate these different kinds of energy on the mesoscopic time scale. The dispersion relation separates the high and low frequencies of motion. As a consequence, the dissipated energy of the high-frequency motions is interpreted as heat energy and attached to the corresponding pair of particles. To
store this information, the particles have an inner variable, describing the corresponding macroscopically observable property temperature $T$. The low-frequency motions instead stay unchanged for long time intervals, compared to the mesoscopic time constant. Depending on the application, additional internal variables like stress or chemical changes can be reasonable or even required.

The standard Lennard Lennard Jones potential is not sufficient to model massive forming processes. These types of systems require the reproduction of additional effects like thermal expansion or local smelting. Therefore Ostermeyer [4] modified the standard Lennard-Jones potential into

$$V_{LJW} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{2n} - \sqrt{1 - \frac{W^2}{\epsilon^2}} \left( \frac{\sigma}{r} \right)^n \right]$$

which explicitly depends on the stored heat energy $W$. This is quite reasonable since the attractive part of the potential vanishes, when the phase transition temperature is reached. $r$ marks the distance between two neighbouring and interacting particles. $\epsilon$, $\sigma$ and $n$ are the potential’s parameters and have to be chosen according to the material properties like Young’s modulus. The inner variable temperature $T$ is connected to the stored heat energy $W$ via

$$W = mc_V T$$

This equation defines heat energy as the product of mass $m$, specific heat capacity $c_V$ and temperature $T$.

In order to achieve the equations of motion of such a particle system, the Lagrangian function $L = E_{kin} - E_{pot}$ is considered with $E_{kin}$ and $E_{pot}$ as the kinetic and potential energies of the given system. $L$ depends on the generalized coordinates $u$ and the generalized velocities $\dot{u}$. The dissipation function $D$ takes into the energy dissipation and only depends on the generalized velocities.

$$\frac{d}{dt} \left( \frac{\partial}{\partial \dot{u}} L \right) - \frac{\partial}{\partial u} L = - \frac{\partial}{\partial \dot{u}} D$$

The total energy inside the system including all the heat energy $W_T$ has to be conserved.

$$E_{kin} + E_{pot} + W_T = \text{const} \implies \frac{d}{dt} (E_{kin} + E_{pot} + W_T) = 0$$

Rearranging this equation yields to the following expression, describing the local heat generation within a system considering heat dependent interaction potentials.

$$\dot{W} = \dot{u} \frac{\partial}{\partial \dot{u}} D \cdot \frac{1}{1 - \frac{\partial L}{\partial W}}$$

To describe the overall local heat evaluation during the forming process, the model does not only have to consider local heat generation but also has to account for global heat conduction (Fourier) within the workpiece and between workpiece and forging die and in addition heat convection and thermal radiation along the surface during the cooling process outside the die. Equation (5) has to be expanded accordingly.
3 MODELLING MASSIVE FORMING PROCESSES WITH PARTICLE METHODS

The modeling of forming processes is very important, since the plastic deformation of a solid body has a significant impact on the final body’s characteristics like strength, strain or vibration resistance. These properties depend e.g. on the evolution of material flow respectively the flow lines during the forming process. The workpiece’s characterics are much better along the flow lines than in a lateral direction.

Before applying a particle method to simulate complex forming processes in order to determine realistic process’ information, the particle model has to be validated. In order to show its reliability, the simulation results of a standard forming process are generated and compared to experimental results. The process, that is going to be analyzed in the following, is the compression of a cylindrical workpiece. The realistic reproduction of this compression is in fact very important, because it oftentimes marks the first forming step within a complex and graduated forming process.

The aspects used to validate the results achieved by the particle method are the flow lines, the temperature distribution and the natural strain that is directly coupled to the microstructural transformation.

The flow line distribution is a result of the grains’ orientation inside the workpiece. Recrystallization leads to a structural change, which is mechanically rearranged during the plastic deformation. The final orientation depends on the initial grain orientation and on the direction of the forming process. FE simulations generate the flowlines by tracking certain grid nodes (the initial coordinates and their displacement evolution) during the forming process. Problems arise, when a frequent remeshing is required, because a new mesh lacks the information on the predestined material flow. The introduced particle method prevents such a loss of information. Each initial flow line is represented by a chain of assigned particles. This initial assignment stays unchanged during the total forming process. The flow line evolution is therefore observed by tracking the assigned particles as part of the corresponding flow line.

The typical vertical and horizontal flow line distribution of such a compression test (experiment cf. [5]) compared to the simulation results is shown in figure 2 and figure 3. The simulation results show the same typical flow line distributions in vertical and horizontal direction as the experiments. The flow lines are parallel to the lateral edges of the final workpiece’s shape. Figures 2 and 3 also show the main advantage of massive formed parts: the typical uninterrupted flow line distribution that allows an excellent behavior considering static and dynamic loading.
The forming process considered is an inhomogeneous one. This means that the deformation is not equal for each point of the workpiece. The result is a convexly compressed workpiece (cf. figures 2 and 3). The reason for this is the amount of friction, that is present between workpiece and upper and lower die respectively plate. This friction prevents an even lateral expension at the workpiece’s end planes. During the forming process, the major fraction of the generated deformation energy is turned into heat energy. As a result of the inhomogenous forming distribution, the temperature distribution as well as the strain distribution are not homogenous either.

Besides the flow lines, the structure (grain size and distribution) has a vital influence on the final workpieces mechanical properties like ductility or further shape cutting. The final grain size of a compressed workpiece depends on the initial grain size, the type of recrystallization (works against the hardening as a result of plastic deformation), the temperature and the natural strain [5]. A larger strain e.g. leads to smaller grains during the dynamic recrystallization. So, for a given initial grain size, the particle simulation has to generate a realistic temperature and strain distribution to deliver the correct final
grain size distribution. That is the reason, why the validation of temperature distribution and local natural or effective strain is essential.

The natural or effective strain distribution describes the amount of local deformation considering the local neighbourhood. The strain distribution after the compression can be experimentally determined by hardness testing. Figure 4 shows the principal strain distribution as a result of experimental Brinell hardness testing [6]. Three different strain areas can be detected: I with large strain, II with medium strain and III with low strain. The area with the highest amount of strain ranges in diagonal form from the center of the workpiece to its edges. The simulation results are in accordance with the experimental observations. The three areas could be clearly identified within the particle representation (cf. figure 4).

![Figure 4: Strain distribution: experimental result (cf. [6]) versus particle simulation result.](image)

The temperature measurement inside the workpiece during and directly after a forming process is not quite possible. So, a comparison between experimental data and simulation results has not been carried out. Instead, figure 5 shows the results of the particle simulation compared to the established ones of an FEM simulation (cf. [6]). These FEM-results show an increase in temperature inside the workpiece that is directly correlated to the strain distribution. Those parts inside the workpiece, that experienced the largest degrees of rearrangement (cf. figure 4) are those with the highest final temperatures after the forming process. As a consequence, the temperature distribution shows a formation of three areas comparable to those of the strain distribution. This correlation is also correctly reflected by the results of the particle simulation.

![Figure 5: Temperature distribution: FEM result (cf. [6]) versus particle simulation result.](image)
The number of particles used for the modelling depends on the system’s size and the required accuracy. The higher the demands on the simulation’s quality respectively the chosen size of potential forming errors are, the smaller will the size of a single particle be, which will result in an increase in the total amount of particles. As the analyzed systems usually have very large numbers of particles, algorithm’s design and the corresponding performance enhancement has become a major task in algorithm development. Parallelization is a widely spread concept for this purpose. The source code parallelization e.g. on multi-core CPUs or CPU clusters is already very popular among scientists and engineers.

During the past few years, another approach allowing massive parallelization on special graphics processing units (GPUs) has been developed by manufacturers like NVIDIA [7]. As a result of the fast growing video game industry, GPUs have been optimized to perform large numbers of floating-point operations for each video frame. Therefore, GPUs allow for a much higher degree of parallelization than CPUs can do. This development is also shown by the fact, that among the top four supercomputers of the world three are already using NVIDIA GPUs [8].

In 2007, only short time after the launch of its first general purpose GPU, NVIDIA introduced a user-friendly computing architecture called CUDA (Compute Unified Device Architecture). This architecture allows standard C programming with additional runtime functions but without dependence on standard graphics user-interfaces like OpenGL anymore.

Besides the performance, GPU Computing has got some other quite important advantages compared to CPU Computing. The acquisition costs per GFLOP as well as the power consumption per GFLOP are much lower for GPUs than for CPUs. The main challenge of GPU Computing is the fact, that CPUs and GPUs require a completely different algorithm implementation. So, a GPU implementation of a given CPU implementation oftentimes results in an algorithm’s redesign. Furthermore, it is the user’s task to generate a workload distribution that leads to an optimal usage of GPU’s resources.

As a matter of principle, GPU computing makes only sense for those systems that provide a large parallel portion in the corresponding algorithm. Systems with no or only minor parallel parts will not benefit from a GPU implementation, quite the opposite. In these cases, a GPU implementation can even worsen the performance. Particle systems e.g. are ideally suited for parallelization, because the same set of instructions has to be executed for each particle. But since the algorithm’s redesign is costly, it has to be determined, if the performance benefit justifies the time and effort.

Therefore, a single CPU (program only executed on one core) as well as a single GPU implementation of the particle system’s update algorithm have been realised for three different types of particle systems as well as an evaluation of the performance [9]. The update procedure is identical for each type of particle system and follows a tree step
update-scheme. The first step includes the determination of each particle’s neigbourhood and is the most time-consuming part of the total algorithm. Therefore the type of interaction detection algorithm has to be well-chosen. Afterwards, the corresponding interaction forces are computed and finally the current set of system’s differential equations is generated and solved via time integration.

The analyzed particle systems vary in system’s size (number of particles) and range of interaction forces. They therefore have quite significant differences in their computational intensities. The variation of the interaction range leads to three different types of particle systems:

- non-interaction particle system: no interaction among the particles; the system’s state update is reduced to the pure time integration
- short-range interaction particle system: particle interaction only within a small neighbourhood; neighbourhood detection, calculation of corresponding interaction forces and time integration required
- all-pair interaction particle system: each particle interacts with all the other particles; no neighbourhood detection required, only brute-force calculation of interaction forces and time integration

As a consequence, the non-interaction particle system has the lowest computational intensity. The all-pair interaction particle system has the highest computational intensity with a computation of interaction forces of order $O(n^2)$. The reduction of interaction range to small neighbourhoods (short-range interaction system) reduces the effort of force calculation to $O(n)$ but requires an additional neighbourhood detection. A variety of neighbourhood detection algorithms (comparable to the problem of collision detection) have been developed [10]. Their efforts vary from $O(n^2)$ to $O(n \log n)$. In contrast, effort’s reduction leads to a rapid increase in memory requirements. Therefore, the neighbourhood detection algorithm, chosen for the following investigations, is the brute-force neighbourhood detection of order $O(n^2)$. It was chosen because it represents a lower limit and so the minimal benefit of performance enhancement of a GPU implementation compared to a CPU implementation for short-range interaction particle systems.

The integration method used is the standard Euler forward integration as it is the basic method. A more time-consuming integration method will lead to similar results since it will affect the implementations on the CPU and on the GPU in a similar way. So, the difference will only be a constant factor. In case of interaction, the particles interact via Lennard-Jones potentials.

The two hardware platforms used for performance evaluation are

- CPU: Intel Core i7-920, 2.70 GHz
- GPU: NVIDIA Tesla C1060 (240 streaming processors)
In order to evaluate the performance of an algorithm implemented and executed on a single CPU core (completely sequential implementation) in contrast to a single GPU implementation (parallelized execution), the computing time required for 100 update steps is measured for both platforms. This time does not consider the time for visualization of the simulation results. If not otherwise indicated, the time required for the GPU implementation does not take into account the time used to copy the data from the CPU to the GPU and finally back to the GPU. The performance is determined by the amount of time, required to complete the update. The more time is spent on the update steps, the slower and therefore worse is the performance of the analyzed implementation.

Figures 6 and 7 show the time in ms required for the GPU and the CPU implementation for the lower and upper limits of computational intensity: the non-interaction particle system and the all-pair interaction system. The blue curve marks the computing time of the CPU implementation and the red curve the one of the GPU implementation.

![Figure 6: Computing time vs. system’s size for the non-interaction particle system.](image)

![Figure 7: Computing time vs. system’s size for the all-pair interaction particle system.](image)

In figure 6, the execution time increases at a constant rate with increasing number of particles for both implementations. This trend was expected, because the non-interaction particle system has a computational complexity of order $O(n)$. In contrast, the all-pair interaction particle system’s complexity of order $O(n^2)$ is directly represented by the CPU implementation (cf. blue curve in figure 7). Figure 7 also shows an important aspect of GPU’s performance enhancement. The GPU implementation reduces the squarish dependency between computing time and system’s size of the sequential implementation.
to a linear one. Although the total time required for the all-pair interaction approach is much higher than the one for the non-interaction system, both systems indicate the same behaviour: the GPU implementation outperforms the CPU implementation for systems larger than a critical system’s size. The critical system’s size is much lower for the computational intensive particle system than for the non-interaction system.

To evaluate the benefit of a GPU implementation in contrast to the CPU implementation, the speed-up is a frequently used quantification value. The speed-up is a factor, that states, how many times faster a GPU implementation is compared to a CPU implementation. It is therefore defined as:

$$\text{speed-up} = \frac{\text{performance}(\text{GPU})}{\text{performance}(\text{CPU})} = \frac{\text{computing time}(\text{CPU})}{\text{computing time}(\text{GPU})}$$

(6)

The speed-up depends in general on the problem’s computational intensity, the degree of parallelizability, the problem’s size and the implementation which requires the optimal usage of GPU’s resources. The amount of information that has to be stored on the GPU for the required computations strongly limits the performance. If large particle systems exceed the GPU’s memory capacities, the particle system has to be manually partitioned by the user and loaded to the GPU and processed sequentially portion by portion. This procedure is necessary since GPUs do not support virtual memory as CPUs do.

Figure 8 shows the resulting speed-ups for the three analyzed types of particle systems. These speed-up results do not represent the highest possible speed-ups comparing single CPU and single GPU implementations, since the implementations have not been optimized to the dead end yet. Instead, the figure should indicate the potential of GPU computing compared to CPU computing. Figure 8 makes clear, that an enormous performance enhancement can be achieved for all types of particle systems, when implementing the algorithm on a single GPU instead of a single CPU.

![Figure 8: Speed-up](image)

It should be noted, that the speed-up also depends on the chosen accuracy. While double and single precision performances do not lead to considerable differences in CPU’s performance, there are large differences in GPU’s performance. The reason for this is the fact, that the older CUDA capable GPUs have only been optimized for single precision.
So the support for double precision operations and performance was neglected, which led to a large performance loss for double precision applications (up to 80% [11]). The new Fermi GPU generation takes care of these insufficiencies and increased not only single but also double precision performance. A double precision GPU implementation is still about 50% slower than a single precision one, but on Fermi GPUs it is able to outperform double precision CPU implementations [12], which was not possible with older GPUs.

5 CONCLUSIONS

- It has been shown, that the modelling of massive forming processes with particle systems delivers a realistic material behaviour considering the evaluated criteria of flow line distribution, strain and temperature distribution. The particle simulation’s results turned out to be in good agreement to the experimental ones and to those of standardized FEM simulations. So, the introduced particle model seems to be qualified to be used for further analysis of more complex forming processes.

- GPU Computing was introduced as a tool for performance enhancement of systems with a large parallel portion. Particle systems meet this demand and are therefore predestined for parallel computing. The analysis of three different types of particle systems showed, that the performance of particle systems’ simulations implemented on a CPU can be improved by parallelizing the neighbourhood detection as well as the state update on a GPU.

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SMOOTHED PARTICLE HYDRODYNAMICS ON GPU COMPUTING

A.J.C. CRESPO*, J.M. DOMINGUEZ*, D. VALDEZ-BALDERAS†, B.D. ROGERS†
AND M. GOMEZ-GESTEIRA*

*Environmental Physics Laboratory (EPHYSLAB)
Universidade de Vigo
Campus As Lagoas s/n, 32004, Ourense, Spain
e-mail: alexbexe@uvigo.es, web page: http://ephyslab.uvigo.es

†School of Mechanical, Aerospace, & Civil Engineering (MACE)
University of Manchester
Sackville Street, Manchester, M60 1QD, United Kingdom
web page: http://www.mace.manchester.ac.uk/

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Abstract. Smoothed Particle Hydrodynamics (SPH) is a powerful technique used to simulate complex free-surface flows. However one of the main drawbacks of this method is the expensive computational runtime and the large number of particles needed when 3D simulations are performed. High Performance Computing (HPC) therefore becomes essential to accelerate these codes and perform simulations. In this study, parallelization using Graphics Processing Units (GPU) is applied to the SPHysics code (www.sphysics.org) dedicated to free-surface flows with SPH. Simulations involving several million particles on a single GPU exhibit speedups of up to two orders of magnitude over the same calculations using CPU codes, while parallelization using MPI for multi-GPU leads to further acceleration. This cheap technology allows studying real-life engineering problems at reasonable computational runtimes.

1 INTRODUCTION

Smoothed Particle Hydrodynamics (SPH) is a purely Lagrangian method developed during seventies (Gingold and Monaghan, 1977) in astrophysics. It has since been developed and applied to a range of engineering flows, in particular for-free surface hydrodynamics problems, such as the study of violent flows, wave breaking, wave-structure interactions.

SPHysics is an SPH numerical model developed to study free-surface flows and is the product of a collaborative effort amongst researchers at the Johns Hopkins University (U.S.A.), the University of Vigo (Spain) and the University of Manchester (U.K.). The open-source code, written in FORTRAN, is available to download for public use at www.sphysics.org. Although the SPH method can provide a fine description of the flow, its main drawback is its high computational cost, so that applying over large domains is prohibitive. Graphics Processing Units (GPUs) are a new technology imported from the
computer games industry that can be used for scientific computing and is ideal for SPH due to its parallel architecture. As a result, the dual functioning CPU-GPU code *DualSPHysics* has been developed using C++ and Compute Unified Device Architecture (CUDA) for operation on CPUs and GPUs, respectively. More information about the *DualSPHysics* project can be found at [www.dual.sphysics.org](http://www.dual.sphysics.org) while different applications and animations can be viewed at [www.vimeo.com/dualsphysics](http://www.vimeo.com/dualsphysics).

In the present work, the *DualSPHysics* solver is presented describing the different parallel codes implemented for different cores of CPU and one or more GPUs. The numerical results are firstly validated with experimental data to show the accuracy and reliability of our scheme, and then the achieved speedups comparing CPU and GPU are addressed to prove the efficiency of this new technology in CFD problems.

## 2 SPH BACKGROUND

SPH is a meshless method that describes a fluid by replacing its continuum properties with locally smoothed quantities at discrete Lagrangian locations and then integrates in time the hydrodynamic equations of motion for each particle in the Lagrangian frame. Relevant physical quantities are computed for each particle as an interpolation of the values of the nearest neighbouring particles, and then particles move according to those values. The conservation laws of continuum fluid dynamics, in the form of differential equations, are transformed into their particle forms by integral equations through the use of an interpolation function that gives the kernel estimate of the field variables at a point. SPH offers distinct advantages including no fixed computational grid being required when calculating spatial derivatives.

The main features of the SPH method, which is based on integral interpolants, are described in detail in Gómez-Gesteira et al., 2010 and Liu and Liu, 2010. Here, only the main points about implementation will be described. Conceptually, an SPH code is an iterative process consisting of three main steps:

a) **neighbour list**: particles only interact with surrounding particles located at a given distance so the domain is divided in cells of the kernel size to reduce the neighbour search to the adjacent cells;

b) **particle interaction**: each particle only looks for neighbours at the adjacent cells, after verifying that the distance between particles lies within the support of the kernel, the conservation laws of continuum fluid dynamics are computed for the pairwise interaction of particles;

c) **system update**: once the forces between neighbouring particles have been evaluated, all physical magnitudes of the particles are updated at the next time step.
3 PARALLEL IMPLEMENTATION OF SPH ON CPU AND GPU

As mentioned, the SPH code is an iterative process where force interactions are computed for all particles and all physical quantities are updated at the following time step. All these tasks are very expensive in terms of computation time when the execution is carried out in a single serial machine, so the parallelization of the tasks for large number of particles becomes imperative. In the particular case of the SPHysics code different parallel techniques have been implemented on different devices, threads of CPU and GPU cards.

3.1 Multi-core implementation using OpenMP

OpenMP, a specification for parallel programming is used to implement the multi-core SPH code. Its implementation is straightforward and no significant changes in comparison to the single-core code are required. Most of the sequential tasks and operations that involve a loop over all particles are performed using the different cores of the same CPU. Thus, the time dedicated to communication between different execution threads is reduced since the same shared memory is used. The code is also optimised with the implementation of dynamic load balancing. As is well known, using OpenMP on its own means that this parallelization and potential speedup are limited to a small number of cores (i.e. the number of cores existing on the compute node).

3.2 GPU implementation.

The GPU parallelisation technique uses the CUDA developed by nVidia. An efficient and full use of the capabilities of the GPU architecture is not straightforward. In this case, the sequential tasks over the particles are performed using different execution threads of the GPU architecture. For example, with a GTX480 card a maximum of 23,040 threads can be executed simultaneously (15 multiprocessors and 1,536 threads per multiprocessor as maximum). The most efficient option is to keep all data in the memory of the GPU where the three main processes of SPH are executed in parallel. The neighbour list follows the procedure used on CPU and some tasks in parallel are even improved by using the optimised radixsort algorithm provided by CUDA. Updating the physical quantities of the particles is easily parallelized. The particle interaction process, which is the most expensive computationally, is implemented solely on the GPU using one execution thread to compute the particle interaction of only one particle. The thread looks for the neighbours of each particle among the adjacent cells and computes the resulting force from all the interactions. Due to the Lagrangian nature of the method, different problems appear such as lack of balancing, code divergence and no perfect coalescent access to the global memory of the device.

3.3 Multi-GPU implementation

Since the memory requirements are still a limitation for a single GPU, using more than one GPU appears to be the best development to continue accelerating SPH simulations. In order to allow different devices communicating with each other, the Message Passing Interface (MPI) is used jointly with CUDA to implement a multi-GPU version of DualSPHysics. MPI presents the advantage of using different compute nodes hosting multiple devices instead of only one.
as it happens with OpenMP. The multi-GPU implementation consists of assigning different portions of the physical system to different GPUs (Valdez-Balderas et al., 2011). After each computation step, data needs to be transferred between devices such as the information of particles that migrate between GPUs (physical sub-domains) or particles that belong to shared spaces where data is used by several GPUs. With the CUDA v4.0, direct GPU-GPU communication is only very recently supported, so the memory transfer between different GPUs is carried out by GPU-CPU, CPU-CPU and CPU-GPU communications which is proving to be 85% efficient without the use of high-speed Infiniband connections to be used in the future.

4 RESULTS

The DualSPHysics code is validated with the same experiment used for the SPHysics validation in Gómez-Gesteira and Dalrymple, (2004) to demonstrate the reliability of the GPU implementation. Thus, model results were compared to experimental data provided by Yeh and Petroff (Chen et al., 1997)) at the University of Washington where a dam break occurred within a rectangular tank, with a volume of water initially contained behind a thin gate at one end of the box and a tall structure was inside the tank. Experimental measurements included the time history of the net force on the structure and the time history of the fluid velocity at a location just in front of the structure. Figure 1 shows different instants of this simulation using one million particles.

![Figure 1: Dam breaking flow impacting on a structure with SPH. Colour represents velocity values.](image)

Figure 2 shows the close agreement between numerical velocity (red line), numerical force (green line) and the experimental values (blue points). The SPH model is able to reproduce the experimental velocity field and the forces generated by the collision between the incoming wave and the structure although the maximum impact force is underpredicted which is most likely due to either the SPH formulation or boundary conditions.
A performance analysis has been carried out for this test case varying the number of particles ($N_p$) and using schemes introduced in Section 3. The codes are executed on the CPU Intel® Core™ i7 940 at 2.93GHz and on the GPU GTX 480 at 1.40GHz. Figure 3 shows the computational runtimes and the number of steps computed per second for the different simulations. Note that $N_{GPU}$ means using $N$ GPU cards while $N_{CPU}$ means running on $N$ cores of the CPU.

The computational runtime increases dramatically with the number of particles when simulations are performed on the CPU device while the GPU technology allows accelerating the code easily even with only one GPU card. In addition, the performance of the GPU, measured here as the number of time steps computed per second is always more than one order of magnitude higher than the performance shown by the CPU codes.

The speedups of using $N_{CPU}$ and $N_{GPU}$ against only one device are shown in Figure 4 to analyse the improvement achieved by using the multi-core and multi-GPU codes respectively. Smaller speedup factors are obtained in the multi-GPU case than in the multi-core approach due to the fact that multi-GPU involves data transferring between different computational devices (GPU to CPU and CPU to CPU), whereas in the multi-core OpenMP approach all data resides in the same compute node, namely, the CPU. Additionally, the multi-GPU scheme does not yet use a high-speed Infiniband connection or feature a load balancing algorithm but the multi-core OpenMP approach incorporates this inherently.
The simulation of one million particles takes more than 2 days on CPU and takes only 55 mins on a single GPU, thus, a speedup of 60 is achieved (Figure 5). The speedups of using \( N_{GPU} \) against \( N_{CPU} \) are also shown in Figure 5 and they are still promising (38-44).

5 APPLICATIONS

In order to create a real complex geometry to reproduce an industrial problem the first main issue is the resolution with which the objects are represented. To obtain realistic results with SPH it is appropriate that the initial geometry is as close as possible to a real industrial problem. This drawback can be solved when several million particles are used in the simulation. Figure 6 shows the example of an SPH simulation for a pump mechanism.
However the main field of application of our software is the design of coastal protection schemes. Simulating million particles in a few hours allows us to investigate a real scenario where the damage due to extreme waves can be analysed and mitigation structures can be designed. Figure 7 shows different snapshots of a simulation where a large wave interacts with an idealised seafront consisting of a beach, a seawalk, pavement, the street, trees and buildings. The model reproduces realistically an overtopping.

**Figure 7**: Promenade-wave interaction with SPH using 20 million particles.

### 6 CONCLUSIONS AND FUTURE LINES

- It is demonstrated that the achieved performance of SPH simulations with a small number of GPUs can be compared to that of large cluster of CPUs, both in terms of speed and in the number of particles employed (Maruzewski et al., 2010). Furthermore, other important advantage is the cost and ease-of-maintenance of GPUs in comparison with those clusters.
- Once the GPU implementation allows studying simulations of large domains with a reasonable computational runtime, real-life engineering problems will be studied for industrial purposes using SPH models.
REFERENCES


A GENERAL COMPARATIVE STUDY IN LONG ROD PENETRATION USING CORRECTIVE SMOOTHED PARTICLE METHOD

A. EGHTESAD *, A. R. SHAFIEI †

* Yazd University
Mechanical engineering department, Iran
e-mail: a.eghtesad@stu.yazduni.ac.ir

† Yazd University
Mechanical engineering department, Iran
e-mail: arshafiei@yazduni.ac.ir

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Abstract. Corrective smoothed particle method (CSPM) has been used to study the dynamic behavior of targets with different materials; AL, ALN and AL-ALN FGM in long rod penetration of an AL projectile. A mixed strength model with sigmoid formulation has been used to describe both yielding and fracture phenomena in the FGM. The strength model includes the JC dynamic yield relation and JHB fracture model with a continuum damage description approach. An efficient renormalization in continuity density approach is used to improve the SPH approximation of boundary physical variables. This study shows that the CSPM method in combination with the proper strength model describing the FGM dynamic behavior, can predict the mixed plastic and brittle response of different materials in long rod penetration problems.

1 INTRODUCTION

FGMs, as a new generation of materials, are widely used in heat barrier systems, aerospace industries and energy absorbing applications. In armor systems, there have been an attempt to predict the dynamic behavior of FGMs under high velocity impact conditions. Recent researches confirm the importance of study of FGMs in the field of dynamic response of materials.

Smoothed particle hydrodynamics (SPH) is a particle and meshless method that has promising advantages in modeling problems with extreme large deformations that include brittle damage and fracture in ceramics. SPH was first proposed to solve cosmological problems in three-dimensional open space such as the simulations of binary stars and stellar collisions [1, 2]. The SPH method has also been applied extensively in computational fluid dynamics related areas that include multi-phase flows [3], incompressible flow simulations [4, 5], free surface flow analysis [6, 7].

In this paper, Corrective smoothed particle method (CSPM) has been used to study the dynamic behavior of targets with different materials; AL, ALN and AL-ALN FGM in long rod penetration problem. A mixed Strength model with sigmoid formulation has been used to
describe both yielding and fracture phenomena in the FGM. Temperature field is evaluated from a heat conduction equation with variable thermal conductivity and the result is used in Johnson-Cook yield model. The presented paper shows that using a functionally graded which macroscopic behavior is described using a sigmoid function, will be resistant enough to penetration of high velocity projectiles. The CSPM method in combination with the proper strength model describing the FGM dynamic behavior, can predict the mixed plastic and brittle response of a ceramic–metal functionally graded material in high velocity impact phenomena and the related fields.

2 SMOOTHED PARTICLE HYDRODYNAMICS

In a SPH formulation, every arbitrary function, \( f(x) \) and its derivative can be expressed using the equations 1, 2, respectively.

\[
  f_i(r) = \sum_j \frac{m_j}{\rho_j} f_j W(r-r_j,h),
\]

\[
  \nabla f_i(r) = \sum_j \frac{m_j}{\rho_j} f_j \nabla W(r-r_j,h),
\]

Where in above equations, \( m_j, \rho_j \) are the mass and density of neighbor particle \( j \), and \( W(r-r_j,h) \) is the kernel function that is covering the support domain with a radius of \( 2h \).

2.1 Continuity equation

The continuity equation in a SPH algorithm can be written as follows:

\[
  \frac{D\rho_i}{Dt} = \rho_i \sum_j \frac{m_j}{\rho_j} (v_i - v_j) \nabla W(r-r_j,h),
\]

Where, \( v_i - v_j \) is the relative velocity between particles \( i,j \).

2.2 Momentum equation

In the absence of the body force, the momentum equation which is commonly used in SPH applications has the following form:

\[
  \frac{Dv_i}{Dt} = \frac{m_j}{\rho_j} \left( \frac{\sigma_{i\alpha}^{\alpha\beta} + \sigma_{j\alpha}^{\alpha\beta}}{\rho_j^2 + \Pi_j} \right) \frac{\partial W(r-r_j,h)}{\partial x^\beta} + \Pi_i.
\]

Where, \( \sigma_{i\alpha}^{\alpha\beta} \) is the total stress tensor with the following relation:

\[
  \sigma_{i\alpha}^{\alpha\beta} = -P \delta_{i\beta}^{\alpha\alpha} + S_{i\alpha}^{\alpha\beta}.
\]

In the above equation, \( P \), is the hydrodynamic pressure, \( S_{i\alpha}^{\alpha\beta} \), is the component of identity tensor, and \( S_{i\alpha}^{\alpha\beta} \) is the component of deviatoric part of stress tensor. The rate of change of deviatoric stress tensor due to time can be expressed as follows:
\[ \frac{D\varepsilon^{\alpha\beta}}{Dt} = 2G \left( \varepsilon^{\alpha\beta} - \frac{1}{3} S^{\alpha\gamma} \varepsilon_{\gamma\gamma} \right) + S^{\alpha\gamma} \Omega^{\beta\gamma} + \Omega^{\alpha\gamma} S^{\beta\gamma}, \]  

(6)

Where, \( \varepsilon^{\alpha\beta} \) is the component of strain rate tensor and is given by:

\[ \varepsilon^{\alpha\beta} = \frac{1}{2} \sum_j \frac{m_j}{\rho_j} \left( (v_j^\alpha - v_i^\alpha) \frac{\partial W(r-r_j,h)}{\partial x_i^\beta} + (v_j^\beta - v_i^\beta) \frac{\partial W(r-r_j,h)}{\partial x_i^\alpha} \right). \]  

(7)

In a same manner, for \( \Omega^{\alpha\beta} \), the component of rotation rate tensor, we have:

\[ \Omega^{\alpha\beta} = \frac{1}{2} \sum_j \frac{m_j}{\rho_j} \left( (v_j^\alpha - v_i^\alpha) \frac{\partial W(r-r_j,h)}{\partial x_i^\beta} - (v_j^\beta - v_i^\beta) \frac{\partial W(r-r_j,h)}{\partial x_i^\alpha} \right). \]  

(8)

In equation (4), the term \( \Pi_{ij} \) is artificial viscosity.

### 3 CSPM CORRECTION ALGORITHM

To reduce the errors in free surface boundaries, a renormalization scheme have been used which is called corrective smoothed particle method (CSPM). CSPM scheme is first proposed by Chen in [8] and specifically is used to normalize the density continuity approach in a SPH algorithm. The CSPM correction can be defined as follows:

\[ \frac{D\rho}{Dt} = \frac{\rho_i \sum_j \frac{m_j}{\rho_j} (v_i - v_j) W(r-r_j,h)}{\sum_j \frac{m_j}{\rho_j} (r_i - r_j) W(r-r_j,h)}. \]  

(9)

### 4 EQUATION OF STATE (EOS)

#### 4.1 Tillotson EOS

The Tillotson EOS was suggested by Tillotson in 1962 [9] for describing the dynamic behavior of metals in high pressures and high rates of plastic strain including phase transition. In this form of EOS, the Hugoniot pressure–volume space is considered to be four distinct regions with the following pressure-density relations in different zones of material:

### 5 DYNAMIC YIELD MODEL

#### 5.1 Johnson-Cook dynamic yield model

The Johnson-Cook dynamic yield model can be expressed as [10]:

\[ \sigma = \left[ A + B e^a \right] \left[ 1 + C \ln^2 \epsilon^* \right] \left[ 1 - T^m \right], \]  

(10)

Where:

\[ T^* = \frac{T - T_{\text{ambient}}}{T_{\text{Melt}} - T_{\text{ambient}}}. \]  

(11)
\begin{equation}
\dot{\varepsilon}^* = \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}.
\end{equation}

$\varepsilon$, $\dot{\varepsilon}$, $\dot{\varepsilon}^*$, $\dot{\varepsilon}_0$, $T$, $T_{\text{ambient}}$, $T_{\text{melt}}$ are the equivalent plastic strain, dimensionless equivalent strain rate, equivalent plastic strain rate, reference equivalent plastic strain rate, ambient temperature and melting temperature, respectively.

6 FAILURE MODEL

6.1 JHB failure model

JHB [11] is a new modification of JH1 and JH2, the two previous failure models offered by Johnson and Holmquist [12, 13]. The advantage of JHB failure model is including a phase change from solid to gas during failure process.

JHB strength model can be written as follows:

For intact material:

$$\sigma = [\sigma_i + (\sigma_{\text{max}} - \sigma_i) \left[ 1 - \exp \left[ -\alpha_i \left( P_i - P_j \right) \right] \right] \left[ 1 + C_{\text{JHB}} \ln \dot{\varepsilon}^* \right].$$

Where:

$$\alpha_i = \frac{\sigma_i}{(\sigma_{\text{max}} - \sigma_i)(P_i + T)}.$$  

In above equations, $\sigma_i$ is the intact stress, $\sigma_{\text{max}}$ is the maximum strength, $P_i$ is the intact pressure, $C_{\text{JHB}}$ is a constant between 0 and 1, $\dot{\varepsilon}$ is the equivalent plastic strain rate, $\dot{\varepsilon}^*$ is the dimensionless equivalent strain rate.

For failed material:

$$\sigma = [\sigma_{\text{max}}^f + (\sigma_{\text{max}} - \sigma_{\text{max}}^f) \left[ 1 - \exp \left[ -\alpha_f \left( P_f - P_f \right) \right] \right] \left[ 1 + C_{\text{JHB}} \ln \dot{\varepsilon}^* \right].$$

Where:

$$\alpha_f = \frac{\sigma_f}{P_f (\sigma_{\text{max}}^f - \sigma_f)}.$$  

7 FGM MIXED PROPERTIES

One of the best methods for defining the macroscopic behavior of a FGM is called sigmoid function [14]. As Chung and Chi have pointed out in [15], the sigmoid function can reduce the stress intensity significantly in the ceramic-metal transition band. The sigmoid function for a plate with thickness of $h$ can be written as:
\[ X(z) = \begin{cases} g_1(z)X_1 + [1 - g_1(z)]X_2, & 0 \leq z \leq h/2 \\ g_2(z)X_1 + [1 - g_2(z)]X_2, & -h/2 \leq z \leq 0 \end{cases} \] (16)

Where, \( X(z) \) is an arbitrary physical property of the FGM (e.g. density, modulus of elasticity, shear modulus). The functions, \( g_1(z) \), \( g_2(z) \), can be expressed using the following relations:

\[ g_1(z) = 1 - \frac{1}{2} \left( \frac{z}{h} \right)^p \quad \text{For} \quad 0 \leq z \leq \frac{h}{2}, \] (17)

\[ g_2(z) = \frac{h}{2} \left( \frac{z}{h} \right)^p \quad \text{For} \quad -\frac{h}{2} \leq z \leq 0. \] (18)

Where, \( P \), is a constant parameter depending on the fabrication process of the FGM. Figure 1 shows the variation of an arbitrary physical property, \( X \), for different values of \( P \), in a sigmoid FGM plate [14].

8 DEFINING THE FGM MIXED STRENGTH MODEL

The most important issue in modeling of a FGM to be as target in an impact problem, is finding a suitable combination of the dynamic yield model for pure metal and failure model for ceramic. In a FGM band, the material is not pure ductile like metal nor brittle like ceramic but is somewhat between them, so, we used the sigmoid function for defining the strength of material in this way:

\[ \text{strength}(z) = \begin{cases} g_1(z)(\sigma_{JC}) + [1 - g_1(z)](\sigma_{JHB}), & 0 \leq z \leq h/2 \\ g_2(z)(\sigma_{JC}) + [1 - g_2(z)](\sigma_{JHB}), & -h/2 \leq z \leq 0 \end{cases} \] (19)

Where, \( \sigma_{JC} \) and \( \sigma_{JHB} \) are the Johnson-Cook yield stress and JHB failure stress, respectively. The functions, \( g_1(z) \), \( g_2(z) \), have the same form of equations 17, 18, respectively.

9 CODE VALIDATION

To validate the CSPM code accuracy, a comparison with experimental data [16] has been done in the present work. In this benchmark, the impact of an AL sphere into an AL plate with initial velocity of 6180 m/s has been simulated. The results show good agreements between the numerical results and experimental data.

The values for crater diameter and length/width ratio of the produced debris behind the target for both CSPM and experimental results have been listed in Table 1.
10 NUMERICAL INVESTIGATION

In this section, a general comparison in dynamic behavior of targets with different materials; AL, ALN and AL-ALN FGM has been done under the impact of an AL long rod penetrator. Long rod penetrator impacts normally into the target with initial speed of 10000 m/s. The penetrator includes total number of 600 particles. FGM target was chosen a rectangle with 8mm width and 20mm height with total number of 4000 particles. Total number of 1280 virtual particles was used for wall boundary particles. Figure 2 shows a schematic view of initial configuration of impact simulation. The initial material properties for AL metal and ALN ceramic have been listed in Table 2. The simulation has been done for $5\mu s$ after impact. Figure 3 illustrates the yield stress, von-Mises equivalent stress, and velocity distribution for AL target in several time steps during the penetration process. Contours of brittle damage, von-Mises equivalent stress, and velocity distribution for ALN and ALN-AL FGM targets, respectively, have been shown in figures 4 and 5 at several time steps. From the results we can conclude that using the FGM target, a smaller crater diameter in input zone of penetration is produced. The plastic deformation of output zone makes less fragmentation than that in the ALN ceramic target.

In the FGM target, less damage and failure can be seen in comparison with the ALN ceramic target. In the ceramic target, there are larger cracks that propagate near the fixed ends, which there is not such a behavior in the FGM target.

Both ALN and AL-ALN FGM targets has a thinner path of penetration than the AL target.

11 CONCLUSION

In the present paper, a corrective smoothed particle method (CSPM) particle method was implemented to study the dynamic behavior of targets with different materials; AL, ALN and AL-ALN FGM in long rod penetration problem. A combination of Johnson-Cook yield model and JHB failure model using sigmoid function was employed to define the strength model of FGM. Temperature field is evaluated from a heat conduction equation with variable thermal conductivity and the result is used in Johnson-Cook yield model. This study shows that the CSPM method in combination with the proper strength model, can truly handle the plastic and brittle response of different materials in long rod penetration problems.

REFERENCES


Table 1: Values for crater diameter and length/width ratio of the produced debris behind the target for both CSPM and experimental results

<table>
<thead>
<tr>
<th></th>
<th>SPH Results</th>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crater Diameter</td>
<td>3.5 cm</td>
<td>3.45 cm</td>
</tr>
<tr>
<td>Length / Width Ratio of</td>
<td>1.4 cm</td>
<td>1.39 cm</td>
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<tr>
<td>Produced Debris</td>
<td></td>
<td></td>
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</table>

Table 2: Initial material properties for AL metal and ALN ceramic

<table>
<thead>
<tr>
<th></th>
<th>AL Material Properties</th>
<th>ALN Material Properties</th>
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</thead>
<tbody>
<tr>
<td>Density (kg / m³)</td>
<td>2710</td>
<td>3226</td>
</tr>
<tr>
<td>Shear Modulus (GPa)</td>
<td>27.1</td>
<td>127</td>
</tr>
<tr>
<td>Melting Temperature (Kelvin)</td>
<td>775</td>
<td>2370</td>
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<tr>
<td>Thermal conductivity (W / mK)</td>
<td>250</td>
<td>18</td>
</tr>
<tr>
<td>Specific Heat (J / Kg °K)</td>
<td>875</td>
<td>880</td>
</tr>
<tr>
<td>A</td>
<td>265</td>
<td>-----</td>
</tr>
<tr>
<td>B</td>
<td>426</td>
<td>-----</td>
</tr>
<tr>
<td>C</td>
<td>0.015</td>
<td>-----</td>
</tr>
<tr>
<td>m</td>
<td>1</td>
<td>-----</td>
</tr>
<tr>
<td>n</td>
<td>0.34</td>
<td>-----</td>
</tr>
<tr>
<td>Kᵢ (GPa)</td>
<td>-----</td>
<td>201</td>
</tr>
<tr>
<td>Kᵥ (GPa)</td>
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<td>260</td>
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</tr>
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<td>Cᵢj\₂ (KPa)</td>
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<tr>
<td>σ_max (GPa)</td>
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<td>Pᵢ (GPa)</td>
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<td>0.1</td>
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</table>
Figure 1: Variation of an arbitrary physical property, $X$, for different values of $P$, in a sigmoid FGM plate [14].

Figure 3: Schematic view of initial configuration of impact simulation
Figure 3: Contour distribution for AL target in several time steps: a) von-Mises equivalent stress (Pa), b) yield stress (Pa) and c) velocity magnitude (m/s)
Figure 4: Contour distribution for ALN target in several time steps: a) von-Mises equivalent stress (Pa), b) Damage and c) velocity magnitude (m/s)
Figure 5: Contour distribution for ALN target in several time steps: a) von-Mises equivalent stress (Pa), b) Damage and c) velocity magnitude (m/s)
DYNAMIC REFINEMENT FOR FLUID FLOW SIMULATIONS WITH SPH

YAIDEL REYES LÓPEZ∗ AND DIRK ROOSE†

∗Department of Computer Science, Katholieke Universiteit Leuven
Celestijnenlaan 200A - bus 2402. 3001 Heverlee, Leuven, Belgium.
Centro de Investigaciones de Métodos Computacionales y Numéricos en la Ingeniería (CIMCNI),
Universidad Central “Marta Abreu” de Las Villas (UCLV)
Road to Camajuaní Km. 5 ½, 54830 Santa Clara, Villa Clara, Cuba.
e-mail: yaidel.reyeslopez@cs.kuleuven.be

†Department of Computer Science, Katholieke Universiteit Leuven
Celestijnenlaan 200A - bus 2402. 3001 Heverlee, Leuven, Belgium.
e-mail: dirk.roose@cs.kuleuven.be

Key words: particle methods, SPH, dynamic refinement, adaptivity

Abstract. In this paper, we present a dynamic refinement algorithm for the SPH method where a particle is refined by replacing it with smaller daughter particles. The position of the new particles is calculated by using a square pattern centered at the position of the refined particle. We propose to reduce the error introduced by the refinement by determining the separation of the pattern and the smoothing distance of the daughter particles such that the kernel gradient error is minimized. The results of the simulations using the fully refined domain and the simulations using the dynamic refinement starting from the unrefined domain are compared and are in a good agreement. Better results are obtained when the proposed method to reduce the error is used.

1 INTRODUCTION

Smoothed Particle Hydrodynamics (SPH) is a fully mesh-free Lagrangian method that has been successfully applied in several types of problems including fluid dynamics and deformation of solids. Using SPH the domain is discretized by a set of particles (or interpolation points) that independently carry the material properties and the local resolution or smoothing distance ($h$) of the particle. Varying the smoothing length allows to vary the spatial resolution. Nevertheless, it is not common in SPH simulations to have different levels of refinement, as in e.g. the Finite Element Method (FEM), to improve the accuracy and/or to reduce computational cost.
The first steps in dynamic adaptivity in SPH were performed for astrophysical simulations, where the density was used as the criterion to change the resolution \cite{1, 5, 6, 11, 14}. In other fields Lastiwka and co-workers \cite{7} proposed a method for adaptively inserting and removing particles and they tested the method in a shock tube problem. More recently, Feldman and Bonet \cite{4} proposed a particle refinement procedure, where daughter particles are located using axis aligned hexagonal and triangular patterns that are scaled according to a spread parameter defined before the simulation starts.

In this paper we present a dynamic refinement procedure in which particles are split based on a velocity criterion. The new “daughter” particles are located in a square pattern centered at the position of the refined particle. The optimal separation of the pattern and the smoothing distance of the daughter particles are determined by minimizing the error produced by the refinement in the gradient of the kernel.

2 SPH Background

The SPH method provides a numerical solution for integral equations and partial differential equations (PDEs). Comprehensive reviews of the method can be found in \cite{8, 9, 12}. Herein we only present the formulation used in this work.

2.1 SPH for general fluid dynamics

Using SPH, the particle approximation of a function is given by

\[
\langle f(x) \rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) W(x - x_j, h),
\]

where \(m_j\) and \(\rho_j\) are the mass and the density of the particle \(j\) respectively, and \(\frac{m_j}{\rho_j}\) approximates the volume of the particle. To approximate the gradient of a function, the following expression is used

\[
\langle \nabla f(x) \rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) \nabla W(x - x_j, h).
\]

The smoothing length \(h\) defines the support domain of the kernel \(W\). Major properties and requirements of \(W\) are summarized and described in \cite{8, 9}. For the simulations presented in this work, a piecewise cubic spline is used as the kernel function.

The SPH approximation, to be applied in general fluid dynamics, is derived by discretizing the Navier-Stokes equations in Lagrangian form. The particle approximation of the density \((\rho)\) is obtained according to the continuity equation using the particle approximation of the velocity gradient plus some transformations, obtaining

\[
\frac{D\rho_i}{Dt} = \sum_{j=1}^{N} m_j (v^a_i - v^a_j) \frac{\partial W_{ij}}{\partial x^a_i},
\]
where \( v \) and \( x \) are the velocity and position respectively (the Einstein notation is applied).

Similarly, the particle approximation of momentum evolution is derived by approximating the stress gradient in the Navier-Stokes momentum equation and applying some transformations. If the viscous part of the stress tensor is neglected and only the pressure is retained then it results in

\[
\frac{Dv^\alpha_i}{Dt} = - \sum_{j=1}^{N} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \frac{\partial W_{ij}}{\partial x^\alpha} + F^\alpha_i, \tag{4}
\]

where \( p \) denotes pressure and \( F^\alpha_i \) represents the external forces.

Although we keep the value of \( h \) fixed for each particle, the dynamic refinement procedure introduces particles with smaller smoothing distance to increase the local resolution. When particles with different smoothing distances interact, it is necessary to symmetrize the interaction between them to avoid a violation of Newton’s third law. Different approaches for preserving the symmetry have been used (see [8]). In this work the smoothing distance used to compute the interaction between particles is modified to produce a symmetric smoothing length using the arithmetic mean. This is, \( W_{ij} = W(x_i - x_j, h_{ij}) \), with \( h_{ij} = (h_i + h_j)/2 \). In the next sections the notation \( W_j(x) = W(x - x_j, h(x) + h_j/2) \) is adopted.

3 REFINEMENT PROCEDURE

In SPH simulations, the finest resolution needed to obtain the required accuracy is commonly used in the whole domain. However, often zones are observed where the flow of the particles is slower and the properties behave smoother. In these zones, fewer particles can be used while a similar accuracy can be achieved. To exploit this, a coarse domain discretization is used at the beginning of the simulation. During the simulation the zones where more particles are needed are identified by using a refinement criterion, and the resolution is locally increased in these zones by applying a refinement procedure.

Refinement is useful only if: (a) there is a gain in execution time compared with the simulation using the fully refined domain; (b) local properties are only slightly changed and global properties like kinetic energy, and linear and angular momentum are conserved; (c) the results obtained using the refinement are an improvement over the results of the simulation using the unrefined domain. Notice that for dynamic refinement the additional computational cost introduced by the refinement procedure has to be carefully considered, since both the identification of the particles to be refined and the procedure to increase the resolution at these particles are performed during the simulation loop.

3.1 Refinement criterion

Several criteria can be used to determine which particles should be refined during the simulation, depending on the type of the problem. Feldman and Bonet [4] used refinement zones, splitting all the particles that move inside those zones. The number of neighbors can also be used and particles with few neighbors can be split to maintain
the local accuracy. Physical properties have been successfully used too as criteria for the refinement. Kitsionas and Whitworth [5, 6] applied a refinement criterion based on a physical requirement known as “Jeans Condition” and Lastiwka et al. [7] used a criterion based on the velocity gradient.

For the simulations in this work, a criterion based on the velocity of the particles is used for dynamic refinement. Particles with a velocity greater than a pre-established threshold are refined. This refinement criterion was found to be adequate in the problems that we considered. Note that the refinement algorithm described below is totally independent of the refinement criterion.

3.2 Refinement procedure

The refinement procedure presented in this work is based on particle splitting, i.e. if one particle \( n \) is selected to be refined, it is replaced by the daughter particles \( d = 1, ..., M \). The properties of these newly introduced particles have to be assigned in a convenient way. Using the continuity density approach, the properties to be assigned are \( (x_d, v_d, m_d, \rho_d, h_d, O) \), where \( O \) represents a set of other properties that depends on the model. Unless there is a physical law that imposes a restriction or condition, the properties should be interpolated to guarantee a smooth representation of the current status of the system in the neighborhood where the refinement takes place.

In this work the position of the daughter particles is calculated by using a square pattern centered at the position of the refined particle. In [15] we studied the possibility of rotating and scaling the square according to the local distribution of the particles in order to reduce the overlap of the newly created daughter particles with the neighbors. This approach introduced additional “damping” in some simulations, and will not be used in this paper. In the next sections we derive an error estimate and a proposal to minimize it.

Similarly to Feldman and Bonet [3, 4], in this work we define two refinement parameters: the separation parameter \( \epsilon \in (0, 1) \) and the smoothing ratio \( \alpha \in (0, 1) \). The first determines the spread of the pattern, i.e. daughter particles are placed in a square with side \( \epsilon d_{\text{ref}} \), where \( d_{\text{ref}} \) is a reference distance, taken to be the initial inter-particle space. The smoothing ratio \( \alpha \) relates the smoothing distances of the daughter particles \( h_d \) and of the original particle \( h_n \) by \( h_d = \alpha h_n \). To determine the final position, the rotation of the pattern has to be decided. In the results presented in this work we use an axis aligned orientation, but a randomly rotated pattern can be used as well.

It was showed in [3, 4] that the only velocity distribution that conserves both linear momentum and kinetic energy is obtained by copying the velocity of the refined particle to its daughters. In addition, a symmetric distribution of the daughter particles and their masses about the original particle position also conserves the angular momentum. In order to preserve these global properties, the velocity of the refined particle is copied to its daughters and the mass is uniformly distributed, i.e. \( v_d = v_n \) and \( m_d = 0.25 m_n \).

The other properties are interpolated at the daughter particle positions. For this
we adopt the Corrective Smoothed Particle Method (CSPM) [2] that provides a particle approximation that has 0th order consistency for both interior and boundary particles [9]. The interpolated properties are calculated according to

\[
f(x) = \frac{\sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) W(x - x_j, h_j)}{\sum_{j=1}^{N} \frac{m_j}{\rho_j} W(x - x_j, h_j)}
\]

(5)

where \(W\) is taken to be the cubic spline.

### 3.3 Refinement error

The refinement procedure modifies the local properties leading to an error in the current status of the system. It is important to have control over the error introduced in order to keep the accuracy of the simulation. In this section we derive a measure for the error using a procedure similar to that of Feldman and Bonet [3, 4], but we focus on the error introduced in the particle approximation of the gradient of a function because the gradient is used in the derivation of the SPH approximation of the continuity and the momentum equation.

Let’s consider the expression given in (2), now taking into account that the symmetrized smoothing distance is used to evaluate the kernel. Although in this work the square pattern is used, we start with the derivation of the error in the general case when a particle \(n\) is refined into \(M\) daughter particles. If the particle \(n\) is refined the approximation of the gradient of a function changes to

\[
\langle \nabla f(x) \rangle^* = \langle \nabla f(x) \rangle - \frac{m_n}{\rho_n} f(x_n) \nabla W_n(x) + \sum_{d=1}^{M} \frac{m_d}{\rho_d} f(x_d) \nabla W_d(x).
\]

(6)

The local error produced at \(x\) due to the refinement of the particle \(n\) can be defined as the sum of the square of the error introduced in each direction of the gradient, i.e.

\[
e_n(x) = \left( \left\langle \frac{\partial f(x)}{\partial x^\alpha} \right\rangle - \left\langle \frac{\partial f(x)}{\partial x^\alpha} \right\rangle^* \right)^2
= m_n^2 \left( \frac{f(x_n)}{\rho_n} \frac{\partial W_n(x)}{\partial x^\alpha} - \sum_{d=1}^{M} \lambda_d \frac{f(x_d)}{\rho_d} \frac{\partial W_d(x)}{\partial x^\alpha} \right)^2,
\]

(7)

where \(m_d = \lambda_d m_n\) and \(\sum_{d=1}^{M} \lambda_d = 1\) to ensure mass conservation, and \(\alpha\) is a summation index that iterates over the component of the gradient according to the Einstein notation.

Now the global error can be written as

\[E_n = \int_\Omega e_n(x) dx.\]

(8)
We will analyze this error for more specific cases.

### 3.4 Density refinement error using the continuity density approach

Using the continuity density approach, more specifically (3), and considering that the velocity of the daughter particles is copied from the refined particle, the local error introduced by the refinement in the approximation of the material derivative of the density is defined by

$$
e_{n}^{\rho} = \langle \frac{D\rho(x)}{Dt} \rangle - \langle \frac{D\rho(x)}{Dt} \rangle^*$$

$$= m_n (v(x) - v_n) \cdot \left( \nabla W_n(x) - \sum_{d=1}^{M} \lambda_d \nabla W_d(x) \right),$$  \hspace{1cm} (9)

from where the global error can be obtained as

$$E_{n}^{\rho} = m_n^2 \int_{\Omega} \left[ (v(x) - v_n) \cdot \left( \nabla W_n(x) - \sum_{d=1}^{M} \lambda_d \nabla W_d(x) \right) \right]^2 dx. \hspace{1cm} (10)$$

Now we can define the following problem:

**Problem 1.** Find \((x_d; h_d; \lambda_d)\), with \(d = 1..M\), such that \(E_{n}^{\rho}\) is minimal.

Since \(E_{n}^{\rho}\) depends on \(v\), which varies in space and time, problem 1 has to be solved each time a particle is refined, which is computationally expensive. Taking into account that the value of the velocities does not change at time \(t\) when the refinement is performed, an approximation of the solution to problem 1 can be obtained by minimizing

$$E_{n}^{\nabla W} = \int_{\Omega} \left( \frac{\partial W_j(x)}{\partial x^\alpha} - \sum_{d=1}^{M} \lambda_d \frac{\partial W_d(x)}{\partial x^\alpha} \right)^2 dx,$$  \hspace{1cm} (11)

which we refer herein as the kernel gradient error.

Still \(E_{n}^{\nabla W}\) depends on \(h(x)\) that also varies in space and time due to the refinement. However, if we fix the refinement parameter \(\alpha\), there are only two possible values for the smoothing distance: \(h_0\), which is the initial value set to the unrefined particles, and \(\alpha h_0\), assigned to the daughter particles. Considering this, the analysis of (11) can be simplified. We take into account two cases: first, \(h(x) = h_0, \forall x \in I_D\), where \(I_D\) is the influence domain of the particle to be refined; and second, \(h(x) = \alpha h_0, \forall x \in I_D\). The solution that gives the smallest values of \(E_{n}^{\nabla W}\) for these two cases can be selected as a good approximation of the solution to problem 1.
3.5 Kernel gradient error using the square pattern.

Using the square pattern, \( \lambda_d = 0.25 \) for \( d = 1..4 \), we determine values for \( \epsilon \) and \( \alpha \) that give a good approximation to the solution of problem 1. Fig. 1 shows the kernel gradient error for different values of \((\epsilon, \alpha)\) for the two considered cases. We should select values for \((\epsilon, \alpha)\) that lead to a small error in both cases, taking into account two more elements: a) if the smoothing distance of the daughter particles is too large too many neighbors would be inside the support domain, which in turn would smooth out the properties of the daughter particles and would increase the computational cost; b) the separation parameter should be chosen to avoid clumped or spaced out distributions. For these reasons we consider that \((\epsilon, \alpha)\) have to be chosen around \((0.5,0.5)\). In this work, we choose \((\epsilon, \alpha) = (0.55, 0.7)\), highlighted with red points in fig. 1.

![Figure 1: Kernel gradient error less than 0.009 for the two considered cases: left, \( h(x) = h_0 \); and right, \( h(x) = \alpha h_0 \). The red points show the position \((0.55, 0.7)\).](image)

4 FREE SURFACE FLOW SIMULATIONS USING DYNAMIC REFINE-EMENT

To simulate free surface flows Monaghan [13] proposed to use the continuity density approach (see eq. 3) together with

\[
\frac{Dv_i^\alpha}{Dt} = - \sum_{j=1}^{N} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} - \Pi_{ij} \right) \frac{\partial W_{ij}}{\partial x^\alpha} + F_i^\alpha, \tag{12}
\]

to evolve the momentum. The artificial viscosity term \( \Pi_{ij} \) is introduced to reduce numerical instabilities that result from the absence of viscous forces in eq. 4. The artificial viscosity is calculated using

\[
\Pi_{ij} = \begin{cases} 
-\alpha c_\mu_{ij} + \beta \rho_{ij}^2 & \text{if } \mathbf{v}_{ij} \cdot \mathbf{x}_{ij} < 0 \\
0 & \text{otherwise}
\end{cases}, \tag{13}
\]
where \( \mu_{ij} = \frac{h v_{ij} \cdot x_{ij}}{x_{ij}^2 + 0.01h^2} \), \( \tilde{\rho}_{ij} = \frac{\rho_i + \rho_j}{2} \), the notation \( A_{ij} = A_i - A_j \) is used, and \( \alpha \) and \( \beta \) are constants that change with the problem.

In [13], an incompressible flow is considered to be slightly compressible. The relative fluctuation in density is proportional to \( \left( \frac{v_{typ}}{c} \right)^2 = M^2 \), where \( v_{typ} \) is the typical bulk velocity, \( c \) is the speed of sound, and \( M \) is the Mach number. The value for \( c \) is chosen to give a density fluctuation of \( \sim 1\% \) resulting in \( M = 0.1 \). To close the system of governing equations the pressure is calculated by applying the equation of state \( p_i = B \left( \left( \frac{\rho_i}{\rho_0} \right)^\gamma - 1 \right) \), where \( \gamma \) is a constant commonly taken as 7, \( \rho_0 \) is the reference density, and \( B \) is a problem dependent constant related with the speed of sound by \( c = \sqrt{\frac{\partial p}{\partial \rho}} \approx \sqrt{\frac{7B}{\rho_0}} \).

### 4.0.1 Breaking dam problem

In the breaking dam problem a 25m side square block of water is considered. Initially the water is at rest in a container until the right wall is removed suddenly. No-slip boundary conditions are applied in solid boundaries using the ghost particle approach (see [8]).

For this problem we study the effect of applying dynamic refinement starting from two different initial discretizations that we call finer and coarser. Then, the results obtained applying the dynamic refinement using \( (\epsilon, \alpha) = (0.5, 0.5) \) and \( (\epsilon, \alpha) = (0.55, 0.7) \) are compared with the results using the corresponding unrefined and fully refined domains.

The simulations for the two different discretizations are set up as follows:

- **Finer discretization.** The unrefined domain has an initial inter-particle spacing equal to 0.833334 that correspond to 900 particles located in a lattice; the fully refined domain is obtained by statically refining the 900 particles to a finer lattice of 3600 particles with an initial inter-particle spacing of 0.416667; the simulations using dynamic refinement start from the unrefined domain and use as the refinement criterion a velocity threshold of \( v_{max} = 10 m/s \).

- **Coarser discretization.** In this case the unrefined domain has an initial inter-particle spacing equal to 1.666667 corresponding to a lattice of 225 particles. As in the previous case, the fully refined domain is obtained by statically refining the 225 particles to a finer lattice of 900 particles with an initial inter-particle spacing of 0.833334 . The simulations using dynamic refinement start from the unrefined domain and use for the refinement criterion a velocity threshold of \( v_{max} = 7 m/s \) \( (v_{max} = 10 m/s \) gives poor results).

Fig. 2 shows the evolution of the particles during the simulations for the finer discretization using dynamic refinement with \( (\epsilon, \alpha) = (0.55, 0.7) \) and using the fully refined

---

1Notice that the fully refined domain corresponding to the coarser discretization is the same as the unrefined domain of the finer discretization.
domain. We observe a good agreement in the distribution and the velocity of the particles. The same occurs in the simulation using $(\epsilon, \alpha) = (0.5, 0.5)$. If the simulations corresponding to the coarser discretization are compared among them in a similar way, the particle distribution and the velocity of the particles are in a good agreement as well.

![Figure 2: Breaking dam simulation.](image)

The evolution of the surge front ($Z$) of the water particles is shown in Fig. 3, where also the experimental result of Martin and Moyce [10] are presented. The values of $Z$ are normalized by the initial value $Z_0 = 25m$ and the time is normalized by $\sqrt{H_0/g}$ with $g$ the gravity force. Contrary to what we expected, the simulation with the lowest resolution gives the results that are closest to the experiment. However, the slower behavior of the surge front in the experimental result could be due to a drag force between the fluid and the bottom which is neglected in the simulations when the free-sleep boundary condition is applied. As was expected, the results of the simulations using dynamic refinement are between the unrefined and the fully refined simulations for both the finer and the coarser discretizations. Despite that the results are very similar, it can be noticed that when using $(\epsilon, \alpha) = (0.55, 0.7)$ the results are closer to the results of the simulation with the fully refined domain than when using $(\epsilon, \alpha) = (0.5, 0.5)$.

### 4.1 Splash of a drop of water

For the simulations of the splash of a drop into rest water, the following situation is considered. A 10$m$ high block of water is at rest in a 25$m$ wide rectangular container, when a water drop with radius 2.0$m$ with center at $(0m, 13.3m)$ and downward velocity of 2$m/s$ starts moving until it splashes into the rest water. Like in the previous problem, no-slip boundary conditions are applied at the solid boundaries.

Four different simulations are performed using a strategy similar to that employed for the breaking dam problem to obtain different resolutions. For the simulation with the unrefined domain 360 particles discretize the rest water and 19 particles the water drop. In the fully refined domain the rest water is discretized by 1440 particles placed in a finer lattice and the drop is discretized by 76 particles. The simulations using dynamic...
refinement start from a discretization of the rest water as in the unrefined domain (360 particles), but using 76 particles to discretize the drop as in the fully refined domain. In the simulations using the dynamic refinement the velocity threshold of the refinement criterion was set to 1.5 m/s.

Fig. 4 shows the evolution of the simulations with dynamic refinement using \((\epsilon, \alpha) = (0.55, 0.7)\) and with the fully refined domain. It can be seen that the movement of the surface as well as the distribution of the velocity are similar. Fig. 5 shows the evolution of the height of the water in each simulation. The simulation with dynamic refinement using \((\epsilon, \alpha) = (0.55, 0.7)\) reproduces very well the wavy behavior of the surface and gives a result that is very close to the result obtained with the simulation using the fully refined domain. Setting the dynamic refinement parameters \((\epsilon, \alpha)\) equal to \((0.5, 0.5)\) leads to a substantial damping of the waves due to a damping of the particle velocities.
5 CONCLUSIONS

We presented a dynamic refinement algorithm for SPH. The refinement parameters, i.e. the separation parameter $\epsilon$ and the smoothing ratio $\alpha$ are chosen such that the kernel gradient error is minimized.

The results for two model problems indicate that using the dynamic refinement procedure, instead of refining the whole domain, allows a substantial reduction in simulation time, while nearly the same accuracy is achieved.

Further issues to be studied are: a) dynamic coarsening, as the opposite of refinement; b) the implementation of the method in 3D; c) the application to other test cases.

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SIMULATING FLUID-SOLID INTERACTION PROBLEMS USING AN IMMERSED BOUNDARY-SPH METHOD

Mohammad Reza Hashemi*, Rouhollah Fatehi† and Mehrdad T. Manzari*

*Center of Excellence in Energy Convergence
School of Mechanical Engineering
Sharif University of Technology, Tehran, Iran

†Department of Mechanical Engineering
School of Engineering
Persian Gulf University, Bushehr, Iran

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Abstract. In this work, the Immersed Boundary Method (IBM) is adapted and implemented in the context of Smoothed Particle Hydrodynamics (SPH) method to study moving solid bodies in an incompressible fluid flow. The proposed computational algorithm is verified by solving a number of benchmark particulate flow problems. The results are also compared with those obtained using the same SPH scheme along with a direct solid boundary imposition technique.

1 Introduction

The rheological characteristics of particulate flows are of prime interest in many industries. These macroscopic characteristics can be described by various hydrodynamic interactions between solids and the surrounding fluid. To investigate such interactions, one needs to accurately determine the hydrodynamic forces exchanged between the fluid and solid bodies.

This paper attempts to numerically simulate particulate flows using a combination of the Weakly Compressible SPH (WCSPH) and the Immersed Boundary (IB) method. The use of immersed boundary method helps to handle problems with solid bodies of complex geometries as reported by Hieber and Koumoutsakos [1]. They used a combination of the IB and the SPH method, however, brought the SPH particles back into an ordered arrangement at the end of each time step. In the present paper, the IB method is used along with a modified scheme of the WCSPH method.

It is known that in the IB method, the portion of the fluid domain confined within solid boundaries, imposes a retarding effect on the motion of solid bodies [2]. This effect leads to an under estimation of the acceleration of the solid bodies. In 2005, Uhlmann [2] proposed
that the momentum of this confined fluid should be taken into account in order to resolve the problem. In this work, this effect is relieved using a momentum rate summation over SPH particles positioned inside a solid body.

In this paper, some modifications are also used in order to improve capabilities of the standard WCSPH method. The so-called Renormalized schemes are used for the first-order and second-order spatial derivatives. Also, the spurious pressure oscillations are reduced using a modified continuity equation.

In the following, first the proposed weakly compressible SPH method is described. This is followed by presenting the direct fluid-solid boundary treatment and the equation of motion of the solid bodies. Next, the IB method and the time integration procedure are briefly described. Finally, the performance of the proposed method is studied by solving migration of a circular cylinder in a shear flow and falling of a circular solid body in a closed channel. Comparisons between the results of the proposed IB-SPH method and those obtained using the same SPH scheme with a direct solid boundary imposition technique, are also performed.

2 The SPH Method

In this work, weakly-compressible laminar fluid flows are considered. The mass and momentum conservation laws give

\[ \frac{d\rho}{dt} = \rho \nabla \cdot V, \]  
\[ \rho \frac{dV}{dt} = -\nabla P + \mu \nabla^2 V, \]  
where \( \rho \) is density of the fluid, \( P \) is pressure and \( V \) is the velocity vector. In order to close this system of equations, a simple equation of state is used as

\[ P - P_0 = c^2 (\rho - \rho_0). \]  

Equations (1) and (2) are solved using the SPH method as discussed below.

2.1 Spatial Derivatives

The numerical approximation of the first derivative, \( \langle \nabla u \rangle_i \), can be obtained as [3, 4]

\[ \langle \nabla u \rangle_i = B_i \cdot \sum_j \omega_j \nabla W_{ij} (u_j - u_i), \]  
where \( W_{ij} = W(|r_{ij}|, h) \) refers to the value of smoothing or kernel function of particle \( i \) at the position of particle \( j \) and \( r_{ij} = r_i - r_j \). Also,

\[ B_i = - \left[ \sum_j \omega_j r_{ij} \nabla W_{ij} \right]^{-1} \]
is a renormalization tensor. Using Taylor series expansion about $r_i$, it can be shown that the method described by Eq. (4) is consistent and converges linearly as $\delta \rightarrow 0$ for a constant ratio $h / \delta [4]$.

A consistent second derivative approximation scheme was recently introduced by Fatehi and Manzari [4] as

$$
\langle \nabla^2 u \rangle_i = \hat{B}_i : \sum_j 2\omega_j e_{ij} \nabla W_{ij} \left( \frac{u_i - u_j}{r_{ij}} - e_{ij} \cdot \langle \nabla u \rangle_i \right),
$$

where the operator ":" denotes the inner product of second-order tensors, $r_{ij} = |r_{ij}|$, $e_{ij} = r_{ij} / r_{ij}$ is a unit vector in the inter-particle direction and $\langle \nabla u \rangle_i$ is computed according to (4). $\hat{B}$ is a renormalization tensor which is computed using the following set of equations

$$
\hat{B}_i : \left[ \sum_j \omega_j r_{ij} e_{ij} e_{ij} \nabla W_{ij} + \left( \sum_j \omega_j e_{ij} e_{ij} \nabla W_{ij} \right) \cdot \hat{B}_i \cdot \left( \sum_j \omega_j r_{ij} e_{ij} \nabla W_{ij} \right) \right] = -I. \tag{7}
$$

These schemes are directly applied to the momentum equation (2). The discretization of the mass conservation equation (1) is described below.

2.2 Modified Mass Conservation Equation

Lee et al. [5] reported that a Weakly Compressible SPH formulation may lead to spurious pressure oscillations. As discussed in [6], a modification to the continuity equation can solve this problem. Here, the mass conservation equation (1) is replaced by [7]

$$
\frac{d\bar{\rho}_i}{dt} = -\rho_i \left[ \langle \nabla \cdot \mathbf{V} \rangle_i + \Delta t \left( \langle \nabla \cdot \langle \nabla P / \rho \rangle \rangle_i - \langle \nabla \cdot \langle \nabla P / \rho \rangle \rangle_i \right) \right], \tag{8}
$$

in which

$$
\langle \nabla \cdot \langle \nabla P / \rho \rangle \rangle_i = \hat{B}_i : \sum_j \omega_j \nabla W_{ij} \cdot \left( \langle \nabla P / \rho \rangle_j - \langle \nabla P / \rho \rangle_i \right), \tag{9}
$$

and

$$
\langle \nabla \cdot \nabla P / \rho \rangle_i = \hat{B}_i : \sum_j 2\omega_j e_{ij} \nabla W_{ij} \left( \frac{P_i - P_j}{\bar{\rho}_{ij} r_{ij}} - e_{ij} \cdot \langle \nabla P / \rho \rangle_i \right), \tag{10}
$$

where $\bar{\rho}_{ij} = (\rho_i + \rho_j)/2$. 

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2.3 Direct Solid Boundary Treatment

Proper evaluation of the hydrodynamic forces is an essential part of simulating particulate flow problems. In the direct treatment of the solid boundaries, the solid boundaries are represented by one layer of SPH particles, as shown in Fig. 1-a, which leads to a fairly smooth and accurate pressure distribution around the solid bodies. To find the pressure and density of a boundary particle, the fluid equation of motion needs to be solved. Adjacent to a solid surface, the momentum conservation equation can be rewritten as

\[ \frac{\nabla P}{\rho} \cdot \mathbf{n} = -\frac{dV}{dt} \cdot \mathbf{n} + \frac{\nabla \cdot \tau}{\rho} \cdot \mathbf{n}, \]  

(11)

where \( \mathbf{n} \) is the unit outward normal to the solid surface. For the boundary particle \( i \), \( \mathbf{n}_i \) can be calculated from the summation of the kernel gradients \([3]\) as

\[ \mathbf{n}_i = \frac{\sum_j \omega_j \nabla W_{ij}}{\sum_j \omega_j \nabla W_{ij}}. \]  

(12)

Discretizing the pressure gradient term in (11) for particle \( i \), leads to

\[ \left( \sum_j \omega_j \frac{P_j - P_i}{\rho_{ij}} \mathbf{B}_i \cdot \nabla W_{ij} \right) \cdot \mathbf{n}_i = -\frac{dV_i}{dt} \cdot \mathbf{n}_i + \left( \frac{\nabla \cdot \tau}{\rho} \right)_i \cdot \mathbf{n}_i. \]  

(13)

The term \( \frac{dV_i}{dt} \) is the acceleration of the boundary particle \( i \) which is evaluated in terms of the predicted acceleration of the corresponding solid body at each time step. Therefore, \( P_i \) can be found explicitly from (13), and \( \rho_i \) is easily updated using the fluid equation of state.
3 Solid Body Equation of Motion

The Newton’s law of motion is used to explicitly update the solid body velocity and position. For a solid body $b$, the linear and angular momentum equations are

$$M_b \frac{dV_b}{dt} = f_b,$$

and

$$I_b \frac{d\Omega_b}{dt} = m_b,$$

where $M_b$ and $I_b$ are the total mass and moment of inertia of the body, respectively, and, $\Omega_b$ is the angular velocity vector. In (14) and (15), $f_b$ and $m_b$ are the hydrodynamic force and moment exerted on the surface of the solid body and are approximated by summations over the boundary particles, as

$$f_b = \sum_j (-P_j n_j + n_j \cdot \tau_j) \Delta S_j$$

and

$$m_b = \sum_j \mathbf{R}_j \times (-P_j n_j + n_j \cdot \tau_j) \Delta S_j,$$

where $\Delta S_j$ denotes a portion of the solid surface. $\mathbf{R}_j$ is the position vector from the center of solid body $b$ as shown in Fig. 1-b. These parameters are associated with the boundary particle $j$.

4 The Immersed Boundary Method

The Immersed Boundary (IB) method was introduced in 1977 [8] in order to impose a complicated no-slip boundary condition. This method can also eliminate the limitations associated with the moving solid boundaries in particle methods [1]. In order to implement the IB method in the context of SPH, considering the idea introduced in [2], the force and moment in the solid body equations of motion (14) and (15) become

$$f_b = \sum_k F_k + \sum_i m_i \frac{dV_i}{dt},$$

$$m_b = \sum_k \mathbf{R}_k \times F_k + \sum_i m_i \mathbf{R}_k \times \frac{dV_i}{dt},$$

where the subscript $k$ refers to boundary points, $i$ stands for the confined SPH particles within the solid body $b$. The second terms in the RHS of Eqs. (18) and (19) resolve the miscalculation of the solid body acceleration. Figure 2 shows a schematic of the interaction forces between the boundary points and the fluid SPH particle.
The interaction forces $F_k$ which act on each boundary point are calculated using the difference between a predicted velocity due to the rigid motion of the solid bodies and the interpolated fluid velocity at the position of the point $k$. The velocity interpolation is done using a kernel function and a summation over the fluid SPH particles $j$ in the neighborhood of the boundary point $k$, as

$$V_k^* = \sum_j c_{kj} V_j^*.$$  \hfill (20)

$V^*$ is evaluated assuming that there is no solid body in the domain and $c_{kj} = \omega_j W_{kj}/\sum_j\omega_j W_{kj}$. Denoting the predicted velocity of the boundary point $k$ by $V_k^d$, one has

$$f_k = \frac{V_k^* - V_k^d}{\Delta t},$$  \hfill (21)

where $\Delta t$ is the time step size. The force acting on the fluid SPH particle $j$ due to the presence of its neighboring boundary points $k$ is

$$F_j = \sum_k c_{kj} F_{kj},$$  \hfill (22)

with

$$F_{kj} = -m_j c_{jk} f_k.$$  \hfill (23)

Thus, the velocity of the SPH particle $j$ should be updated as

$$V_j = V_j^* + \Delta t \frac{F_j}{m_j}.$$  \hfill (24)

Finally, $F_k$ is calculated as

$$F_k = -\sum_j c_{jk} F_{kj}.$$  \hfill (25)
It must be noted that the only difference in using the IB technique in combination with the proposed SPH method is that equations (16) and (17), which are calculated using the direct solid boundary treatment method, are replaced by Eqs. (18) and (19).

5 Time Integration

To solve the governing equations in time, a two-step predictor-corrector method is used. First, velocity $V^*$ and density $\rho^*$ are predicted solving the equations of motions. Then, the pressure field is updated using $\rho^*$ in (3). Next, the corrected values $V^{**}$ and $\rho^{**}$ are calculated, solving flow equations using the predicted ($^*$) values. The new values of velocity, density, and position are then computed sequentially using

$$V^{n+1} = \frac{1}{2} (V^{**} + V^*),$$

$$\rho^{n+1} = \frac{1}{2} (\rho^{**} + \rho^*),$$

and

$$r^{n+1} = r^n + \Delta t V^{n+1}.$$  

Here, $\Delta t = t^{n+1} - t^n$ and after stability analysis one finds that $\Delta t$ must be constrained by [9]

$$\Delta t = \alpha \min \left( \frac{\delta_{\min}}{U_{\max}}, \frac{\rho \delta_{\min}^2}{\mu} \right).$$

Here, $0 < \alpha < 1$ is a constant, $\delta_{\min}$ is the minimum distance between two neighboring SPH particles, $U_{\max} = c + V_{\max}$ is the maximum characteristic velocity, $c$ is the speed of sound which appears in (3) and $V_{\max}$ is the maximum velocity of the SPH particles. It must be noted that, both linear and angular velocities of the moving solid bodies are also updated, using (14) and (15) in every predictor and corrector steps and finally averaged in the same way as the fluid SPH particles.

During a SPH simulation, defects may be produced by non-uniform distribution and clustering of SPH particles. To alleviate this problem, Xu and his co-workers proposed a particle shifting defined by $\delta r_i$ [10] as

$$\delta r_i = \beta V_{\max} \Delta t \sum_j \frac{r_{ij}^2}{r_{ij}^2} e_{ij},$$

where $r_i = \frac{1}{N_i} \sum_j r_{ij}$, and $N_i$ is the number of neighboring particles for particle $i$. The constant $\beta$, should be within the range $0.001 - 0.1$ to prevent numerical instability and large errors [10]. In this work, the same modification is used in the context of Weakly Compressible SPH (WCSPH) method.
6 Results

In this section, the proposed method is verified by solving two planar low-Reynolds benchmark problems. First, the migration of a neutrally buoyant solid body in a shear flow is simulated, and secondly, the problem of a falling solid body under the effect of gravity force, in a closed channel is solved. For all simulations, a Quintic Wendland kernel function [11] is used with a cut-off distance $h$ of 2.6 times the initial SPH particle spacing, $\delta_0$. The sound speed $c$ in (3) is chosen to be almost 20 times the maximum velocity in the domain to ensure the incompressibility condition [12] and the constant $\alpha$ in (29) is set to 0.5.

6.1 A Neutrally Buoyant Circular Cylinder in a Shear Flow

In this problem, a neutrally buoyant rigid circular cylinder is free to move in a shear flow as shown in Fig. 3. The height of the channel, $H$, is 0.01(m) and the ratio of solid body radius to the channel height is $R/H = 1/8$. The velocities of the upper and the lower walls are equal to $U_w/2 = 0.01(m/s)$ in opposite directions. The particle Reynolds number, $Re_p = U_wR^2/\nu H$, for which the results were reported in [13], is 0.625. The solid body is initially at rest positioned at $y = 0.75H$. The left and right sides of the channel are periodic boundaries.

Here, the length to height ratio of the channel, $L/H$, is set to 5, which ensures that results are independent from the chosen channel length. Also, $\beta = 0.01$ and $c = 0.25(m/s)$. In Fig. 4, the vertical positions of the solid body is shown in time, for both the direct solid boundary treatment and the IB method. The results are compared with those reported by Z-G Feng [13] in 2002. In this problem, the initial SPH particle spacing is $\delta_0 = 1/6000(m)$. It is observed that the result obtained using the WCSPH method is almost the same as those shown in [13]. However, for the IB method some oscillations occur when the solid body reaches the centerline of the channel.

6.2 Falling of a Circular Cylinder in a Closed Channel

In this problem, a circular cylinder starts to move from rest under the gravity effect, with $g = 9.81(m/s^2)$. A schematic geometry of the problem is shown in Fig. 5. The
domain dimensions are $H = 0.06\,(m)$ and $L = 0.02\,(m)$, the radius of solid cylinder $R = 0.00125\,(m)$ and the center of the solid is initially at $x = 0.01\,(m)$ and $y = 0.04\,(m)$. The solid and fluid densities are, respectively, $\rho_s = 1250\,(kg/m^3)$ and $\rho_f = 1000\,(kg/m^3)$, and the fluid viscosity is $\mu = 0.01\,(Pa\,s)$.

Here, $\beta = 0.02$ and $c = 1.0\,(m/s)$. In Fig. 6 the calculated vertical velocities of the falling solid body, for both the direct solid boundary treatment and the IB method, are compared with the result reported in [14]. In this problem, the initial SPH particle spacing is $\delta_0 = 1/10000\,(m)$. Although the results are in good agreement, some oscillations appear in the velocity when the solid body reaches its terminal velocity. These occur as a result of small pressure oscillations imposed by the pressure waves produced in a weakly compressible fluid. In this problem, the acceleration of the solid body changes from the gravity acceleration at the beginning to zero when a terminal velocity is achieved. Thus the performance of the solid boundary treatment methods can be assessed. While the solid body is falling with a variable velocity, the direct boundary treatment method performs better. On the other hand, when the solid body reaches its terminal falling velocity, the results obtained using the IB method are in a better agreement with those reported in [14].

7 Conclusion

Both direct solid boundary treatment and the IB method performed well in particulate flow simulations. However, the results obtained using the direct boundary treatment method were in a better agreement with the results available in the literature while the solid body was moving with a variable velocity. On the other hand the IB method gave
Figure 5: Schematic diagram of the falling circular cylinder in a closed channel.

Figure 6: Vertical velocity of the falling particle in a closed channel in comparison with [14].
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a more accurate result at the terminal velocity.

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This volume contains the Full Papers accepted for presentation at the II International Conference on Particle-based Methods (PARTICLES 2011) held in Barcelona, Spain on October 26-28, 2011.