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ECCOMAS NEWSLETTER - NOVEMBER 2011

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FORWARD

The calendar of ECCOMAS in the odd years is marked by the organization of Thematic Conferences and by the preparations for the global ECCOMAS event the following year. This year 24 Thematic Conferences have taken place in different parts of Europe. The Thematic Conferences cover a broad range of cutting edge topics in Computational Methods in Applied Sciences and Engineering with an estimated attendance for this year of over 5000 participants. A very promising ingredient of these conferences, which is also observed at the global ECCOMAS congresses in recent years, is their appeal to the young generation of researchers whose participation was greatly increased at these events. This participation is encouraged by the financial support provided by ECCOMAS to a large number of young investigators for travel and subsistence expenses.

The First PhD ECCOMAS Olympiad was inaugurated this year, opening a forum for exchanging new ideas, disseminating recent developments and sharing common research interests, among young investigators whose PhD thesis was approved by a University or Research Organization in Europe during the previous year.

The ECCOMAS Congress on Computational Methods in Applied Sciences and Engineering, to be held in Vienna in September 2012, has already attracted the interest of many researchers from around the world, as it is witnessed by over 120 Mini-Symposia approved for organization by distinguished researchers on a large variety of topics. Next year, another ECCOMAS event addressed to young investigators will also take place: The ECCOMAS Young Investigators Conference on Computational Methods in Applied Sciences (YIC 2012) to be held in Aveiro, Portugal, which intends to be a privileged forum of discussion and interchange of ideas by PhD students, Post Docs and young researchers under the age of 35 from European countries as well as from countries all over the world.

This electronic edition of the ECCOMAS Newsletter contains an article by A. Boudouvis et al. on a computational framework for multiscale analysis of chemical vapor deposition processes for the production of films utilized on semiconductor devices, micro- and non-electromechanical systems and protein microarrays and chips, among others (pages 5–9). Summaries of the two best PhD theses, selected for the year 2010, are presented by the two award winners, D. Kah and F.P. van der Meer. The theses are entitled “On the effort of polydispersity for the modeling of liquid fuel injection in internal combustion engines” (pages 13–16) and “On the computational modeling of failure in composite laminates structural materials” (pages 10–12), respectively. This issue also contains the Laudatio addressed by P. Wriggers at the Honorable Colloquium devoted to Professor E. Stein for his 80th birthday (pages 4–5), as well as a report by N. Lagaros on the First Olympiad which took place in Athens in June 2011 (page 22).

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Laudatio for Professor E. Stein on the Occasion of his 80th Birthday Addressed at Honorable Colloquium

His fields of activity are numerous and different. There is the successful researcher and teacher Professor Stein who was honoured many times as well national as international. There is the Civil Engineer who approved many complex buildings in Hannover and the former editor of the German journal "Bauingenieur". At last Prof. Stein is the leading figure of the Leibniz exhibition shown many time in Germany and abroad.

Prof. Stein was born in 1931 in Altendiez/Lahn. From 1951 to 1958 he studied Civil Engineering and Mathematics at the Technical University of Darmstadt where he obtained the degree "Diplomingenieur". After that he worked for one year as a structural engineer in a consulting company. He then accepted a position as scientific assistant at the University of Stuttgart where he finished his PhD on "Treffitz-method for beams, plates and shells" in 1964. After that he worked on his Habilitation that resulted in a contribution on "Coupling of FEM and extended Trefftz method for plates and shells" in 1969. In 1971 E. Stein was appointed to the chair for Structural Mechanics at the University of Hannover that he held for almost 30 years until his retirement in 1998. Additionally he was awarded the position as official inspection engineer of Structural Engineering in the State of Lower-Saxony in 1973. In 1981 Prof. Stein initiated a DFG-Research priority program on "Non-linear Computations in Structural Engineering" which brought researchers from many different German schools together and can be viewed as a starting point for modern Computational Mechanics in Germany. At the same time he applied successfully for a scientific GAMM committee on "Discretisation Methods in Solid Mechanics" with the goal to bring mathematicians and engineers together for interdisciplinary research projects. This committee was a great success and existed almost 20 years. Prof. Stein is also a founding member of IACM and acted since the foundation of GACM as vice-president for 10 years. Prof. Stein contributed not only to the German Computational Mechanics group very strongly he is also president of the ECCM and thus has a lasting influence on the development of the field in Europe within ECCOMAS.

His scientific achievements are represented in 310 publications on physical and mathematical modelling, mathematical and numerical analysis, numerical algorithms and software engineering in continuum and structural mechanics. This work has been honoured by different organizations. In 1993 Prof. Stein obtained the Max Planck Research Award together with Professor Piotr Perzyna of the Polish Academy of Sciences from the Alexander von Humboldt-Foundation and the Max Planck Society. He received honorary doctoral degrees from the University of St. Petersburg in Russia, Poznan in Poland, the China University of Mining and Technology at Xuzhou and Beijing in China and the University of Stuttgart in Germany. He was awarded in 1998 with the highest honor of IACM, the Gauss-Newton medal. He is member of the Braunschweigisch Wissenschaftliche Gesellschaft, the Leibniz Society in Hannover, member of the International Society for the Interaction of Mathematics and Mechanics and corresponding member of the Austrian Academy of Sciences in the class of Mathematics and Natural Sciences and member of numerous editorial boards of international journals.

Prof. Stein has guided 50 PhD students and initiated over 10 habitations. Many of his former students hold now chair positions at Universities or are professors at universities of applied sciences which again reflects the impact of the scientific work of Prof. Stein on the German community of Computational Mechanics.
Since 1990 Professor Stein developed new interest by researching the life of the universal genius Leibniz. He designed the Leibniz exhibition together with Prof. Lindinger under the motto “Gottfried Wilhelm Leibniz – way ahead of his time – Philosopher, Mathematician, Physicist and Engineer”. His research on the calculating machine of Leibniz lead to a new working model and was honored by the DFG in 2005 with the “Von-Kaven-Förderpreis Mathematik” for instrumental mathematics.

The leitmotifs of Leibniz “theoria cum praxi” and “commune bonum” guide also Erwin Stein’s journey through life. We wish him physical health and many more years for his research in the field of Computational Mechanics and on Leibniz.

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A COMPUTATIONAL FRAMEWORK FOR MULTISCALE ANALYSIS OF CHEMICAL VAPOR DEPOSITION PROCESSES

INTRODUCTION

The produced films via chemical vapor deposition (CVD) are utilized to a wide range of applications; from semiconductor devices to micro- and nano-electromechanical systems (MEMS and NEMS), and protein microarrays and chips. Nowadays, the size of these devices or systems shrinks to lower scales and the specifications of the films, e.g. thickness, conformity (thickness uniformity on a patterned surface), surface morphology, refer to properties in micro- or nano-scale. Thus, the single scale conventional CVD modeling methods are not adequate and more advanced, multiscale modeling, methods are needed for studying the phenomena in the co-existing (multiple length) scales. For example, the filling of a micro-trench on the wafer and the pertinent film conformity come from the “interaction” of the macro- or reactor scale with the micro- or feature (trench) scale (Figs. 1a, 1b and 1c). Similarly, the nano-roughness developing on a film’s surface during deposition comes from the interaction of the macro- or reactor scale with the submicro- or nano- or surface morphology scale (Figs. 1a and 1d).

The description of each scale requires a model: The reactor scale model (RSM) is used for the description of the transport phenomena in the bulk phase of the CVD reactor, the feature scale model (FSM) is used to describe the film deposition inside the features (e.g. trenches) and the nano-morphology model (NMM) is used to trail the surface morphology of the deposited film. The effect of the operational parameters of a CVD reactor on the film profile evolution inside a trench on the wafer or on the film’s surface nano-morphology evolution can be predicted by linking or coupling of RSM with FSM or NMM. The linking of models refers to their sequential use, while the coupling

Figure 1. The length scales of a CVD process.

(a) CVD reactor (macro-scale). (b) A cluster of trenches on the wafer. (c) A trench of the cluster (micro-scale). (d) Rough surface of a film deposited on an initially flat surface (submicro- or nano-scale).
incorporates a two-way interaction of the models.

In the following sections, a multiscale computational framework is described and applied to CVD of a film on a predefined topography, i.e. an array of trenches on the wafer; the latter computations require the coupling of RSM with FSM. Additionally, the framework is applied to CVD of a film on an initially flat wafer; linking of the RSM with NMM is performed to calculate the surface morphology of the deposited film.

**THE MULTISCALE COMPUTATIONAL FRAMEWORK**

The multiscale computational framework consists of an RSM, a FSM, a NMM and the algorithms for coupling RSM with FSM and linking RSM with NMM.

The **RSM describes the transport phenomena in the macro-scale of the CVD reactor.** The governing equations are the continuity, the momentum, the energy and the species transport equations [1,2]. They are solved numerically at steady state to predict the velocity, pressure, temperature and species concentrations inside the bulk phase of the CVD reactor. The CFD code Ansys 12 / Fluent [3] is used for the numerical solution of the aforementioned set of equations.

The **FSM results from coupling [4,5] a local flux calculation model, a surface model and a profile evolution algorithm.** The local flux calculation model is a ballistic model [6], which is formulated by a set of integral equations [7] and it is valid at the high Knudsen number conditions occurring in the micro-trenches of the predefined topography. It links the fluxes of the species arriving just above the predefined topography on the wafer with the local fluxes inside the features (e.g. trenches) of the topography. The surface model describes the surface processes and quantifies the effect of species’ fluxes or concentrations on the local deposition rate. The profile evolution algorithm of the deposited film inside the features (moving boundary) uses the level set method [8].

The **NMM is based on the kinetic Monte Carlo method [9,10].** All surface processes, i.e. adsorption, surface diffusion, surface reaction, desorption are modeled as a Markov process by transition probabilities per unit time. The transition probabilities per unit time are modeled by an Arrhenius expression and depend on local activation energies. The NMM is essentially a surface model as the surface model of the FSM; however, the surface model of the FSM is formulated by an analytical surface reaction rate expression (e.g. in terms of the reactive species concentration) and cannot predict the surface morphology. The NMM can also “operate” at sub-micro- or even at micro-scale by the implementation of specific coarse grained methods [10].

The **coupling of the RSM with FSM** is based on [1] the correction of consumption rates of each species on a predefined topography (e.g. an array of trenches) on the wafer. The aim of this correction is to take into account the increased consumption of species inside the topography, without the topography being included in the computational domain of macro-scale. A correction factor, $\epsilon_k$, is applied to each surface reaction rate $k$, reflecting a change of the boundary condition of the species equation. The coupling methodology [1] starts with the numerical solution of the equations of the RSM. Effective (i.e. implicitly taking into account the topography on the wafer) reaction rates are calculated $r^S_{\text{micro},X}(\epsilon_x)$. The density, $\rho$, the temperature, $T$, and the mass fractions, $\omega_i$, for all species are fed to FSM, which in turn computes the local reaction rates inside the features and consequently the average reaction rates $r^S_{\text{macro},X}(\epsilon_x)$; $\epsilon_x$ is then corrected through a fixed point iteration scheme and returned to RSM. The superscripts $(n+1)$ and $(n)$ correspond to two successive steps of the iterative procedure; $\epsilon_x$ is corrected until $r^S_{\text{macro},X}(\epsilon_x)$ and $r^S_{\text{micro},X}(\epsilon_x)$ are equal.

The procedure is applied locally along the wafer radius, or in computational terms, on all the boundary cells of the RSM of the wafer (see Fig. 2). After convergence of the iterative scheme, film profile evolution inside the features is performed for a time step. The same procedure is followed for all time instances. The change of the film profile inside trenches alters the available for deposition surface area and modifies the consumption of each species on the wafer.

The **linking of the RSM with NMM** starts with the numerical solution of the equations in the macro-scale at steady state. All species fluxes just above the wafer are fed to NMM. No bidirectional exchange of computational information between the scales is performed. In other words, no effect of the nano-scale on the macro-scale is considered. This is a reasonable assumption given that the change of the surface nano-morphology is not expected to alter the species consumption on the wafer surface.

**PARALLEL PROCESSING**

The computations in the micro-scale (FSM) can be performed independently at positions along the wafer radius or at the boundary cells of the RSM. The latter is exploited in the proposed coupling methodology by using a synchronous “master–worker” parallel
computational technique. Message passing interface (MPI) is used for the exchange of computational information between the processors. The “master” node in this work is the processor responsible for executing RSM. The computational load, i.e. the computations of FSM at each boundary cell, is partitioned to the processors, the “workers” (Fig. 2). Each processor handles the computations for one or more boundary cells. Each processor accesses only the information needed for its assigned problem. RSM is idle during the computations in the micro-scale. When the computations in the micro-scale are finished, the “master” processor is responsible to gather all the information from all the other “workers” and return it to RSM to continue the computations in the RSM [11].

### Results & Discussion

In this work, results regarding two well studied cases are presented: CVD of tungsten (W) from WF$_6$ and H$_2$ and CVD of silicon (Si) from SiH$_4$. Details for the gas phase and surface kinetics can be found in Refs [1] and [12]. The reactor is a vertical, stagnation point, cold-wall CVD reactor with axial symmetry (Fig. 2a).

**Figure 2.** Schematic of the parallel implementation of the coupling methodology between RSM and FSM. (a) CVD reactor. (b) Boundary cells at the top of clusters of features. The computations in each boundary cell are assigned to one processor. $A_i$ is the total surface of the features in the cluster. $A_{bc}$ is the surface of the boundary cell through which, information is transferred from the macro- to the micro-scale [i.e. mass fractions, density, and temperature $(\omega_{ij}, \rho_j, T_j)$] and vice versa [correction factor $(\varepsilon_{kj})$].

**Coupling of RSM with FSM**

The importance of the feedback from the micro- to the macro-scale is demonstrated in Figs. 3a and 3b. In both figures the film profile of W in a trench at a specific position along the wafer radius is shown: Non-uniform deposition (non-conformal film) occurs and a void is formed inside the trench. The conditions under which both figures are produced are the same. The only difference is that in Fig. 3b no feedback from the micro- to macro-scale is performed, i.e. only linking, and not coupling, between the RSM and FSM is performed. Only linking leads to an overestimation of the deposition rate.

**Figure 3.** Results of coupling RSM with FSM: W and Si film profiles deposited in a trench of a predefined topography on the wafer. a) W profile in a trench belonging to a cluster of trenches extending from 0.045 m to 0.05 m from the center of the wafer. The density of trenches on the wafer is uniform and equal to 8 trenches per 32 μm. The initial width and depth are 1 μm and 1.5 μm. Pressure is 133 Pa. The feed of the reactor is 1 sccm of WF$_6$, 199 sccm of Ar and 1000 sccm of H$_2$. The wafer temperature is 673 K. The deposition time is 15000 s. b) The same as (a) when linking between RSM and FSM occurs, i.e. without feedback from the micro- to the macro-scale.

c) The same as (a) but with a different density of trenches on the wafer, namely 2 trenches per 32 μm.

d) Si profile in a trench belonging to a cluster of trenches extending from 0.0600 to 0.0624 m from the center of the wafer. The density of trenches on the wafer is uniform and equal to 8 trenches per 32 μm. The initial width and depth are 1 μm and 3 μm. Pressure is 133 Pa. The feed of the reactor is 1000 sccm of SiH$_4$ and N$_2$ with the SiH$_4$ mole fraction is 0.1. The wafer temperature is 1050 K.

e) The same as (d) but with a different feed: the SiH4 mole fraction is 0.001.
profile in the same trench and under the same operating conditions of the reactor as in Fig. 3a is shown. The difference is the lower density of trenches on the wafer (2 trenches per 32 μm instead of 8 trenches per 32 μm in Fig. 3a) which means lower available-deposition area. The thickness of the film is greater in the case of the lower density because the local deposition rate is greater.

In Figs. 3d and 3e the effect of an operational parameter on the film conformity during CVD of Si is demonstrated. In Fig. 3d the film profile of Si in a trench at a specific position along the wafer radius is shown. If the SiH₄ mole fraction at the inlet of the reactor decreases, then the deposition is less uniform, the void is larger, as shown in Fig. 3e. The origin for the non-uniform deposition is the increase of effective sticking coefficient of SiH₄ [12].

The effect of a predefined topography on the deposition rate and the gas phase composition is demonstrated in Fig. 4. In Fig. 4a the average deposition rate of Si in a predefined topography of trenches is shown versus the deposition time. At t=0 the trenches are empty (Fig. 4c). Compared to the case of a flat wafer surface with no topography, the available for deposition area is greater and the consumption of the reactants (SiH₄ and SiH₂) on the wafer is also greater. The increased consumption yields to a depletion of the reactants close to the wafer (see the mole fraction of SiH₄ in Fig. 4b) and a decrease of the deposition rate. As the time elapses, the trenches fill and after their repletion (see Fig. 4e) the deposition rate approaches the deposition rate on a flat wafer surface. Additionally, after the repletion of trenches, the composition in the gas phase approaches the composition in the gas phase of a wafer without topography.

**Linking of RSM with NMM [12]**

The results concern the epitaxial deposition of a crystalline film of Si on a Si(001)×1 surface where dimmers are formed [13]. A simple model for the local activation energies is adapted [14] which implements an anisotropy of the surface diffusion and eventually an oriented deposition mode. In particular, the clusters formed on the surface exhibit two alternate orientations on successive deposited monolayers. Simple-cubic lattice with first nearest-neighbor interactions and the solid on solid approximation are considered. In Fig. 5a the surface morphology at the center of the wafer after deposition for 1.5 s is shown. In Fig. 5b the same is shown at the edge of the wafer. The center and the edge positions correspond to the maximum and minimum deposition rate as computed by the RSM. Due to the difference in the deposition rates the number of monolayers deposited differs and leads to surfaces with different cluster's orientation.

Summarizing, a computational framework implementing multiscale modeling of CVD processes is presented. It can couple the macro- with the micro-scale of a predefined topography on the wafer and the macro- with submicro- or nano-scale
of the surface morphology of a film deposited on an initially flat wafer. The acceleration of the computations by parallel processing makes this framework a real enabling tool for studying physics. Following the requirements for models and coupling algorithms linking the operational parameters of the reactors with properties in the nano-scale [15], the next step is to couple all scales (macro-, micro-, and nano-). The current application of interest is metal-organic CVD, and in particular aluminum and copper CVD inside a micro-topography on the wafer. The aim is to investigate the origin of roughness developed inside the micro-topography.

REFERENCES


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Introduction

Laminated composites are attractive structural materials for their excellent strength-to-weight and stiffness-to-weight ratios. They derive these good properties from their microstructure, consisting of stiff and strong fibers and a polymer matrix. However, the importance of the microstructure complicates the understanding of failure of laminates.

Laminated composites are essentially multiscale materials (see Figure 1). Different failure processes, originating from the microstructure may occur and interact to constitute global macroscopic failure (see Figure 2). The failure process that generally occurs first is matrix cracking, which is also, and particularly when the crack is in load direction, referred to as splitting. Matrix cracks are oriented through the thickness of the individual layer, or “ply”. Furthermore, they are straight because they run between the straight fibers.

Another failure process is cracking between the plies, or “delamination”. Delamination may initiate where stress concentrations exist on the ply interface. This can be near the free edge, due to differing contraction properties of the different plies, as well as near matrix cracks, where stress is transferred to from the cracked ply to its neighbors.

In different tests, extensive matrix cracking and delamination has been observed before the peak load of the specimen was reached. The load is redistributed over the fibers as this subcritical damage develops. Eventually, the stress in the fibers will reach the fiber strength at which point fiber failure occurs. Often, onset of fiber breakage is the equal to global failure of the specimen.

In order to predict laminate failure computationally, it is crucial to combine realistic representations of the different failure processes in a single robust framework.

Ply Failure

Failure of the ply can be subdivided into matrix failure and fiber failure. Continuum models have been developed for the single ply in which two independent damage variables are used to distinguish between the two different processes, each with its own stiffness degradation scheme. However, there is a fundamental problem with the continuum approach to matrix failure, namely that localization is not enforced to be aligned with the fibers as it is for real matrix cracks [1]. Another way to view this problem is that no distinction can be made between the stress-strain response for a $u_{1x2}$ deformation and a $u_{2x1}$ deformation, while in the real material only the first leads to a matrix-failure-only failure mechanism of the single ply (see Figure 3).

Therefore, it is to be preferred to represent matrix cracks in a discontinuous fashion. It is proposed to do this with XFEM, because this avoids the need to accommodate the cracks a priori in the mesh [2]. A cohesive model is used for crack growth, where the fact that the cracks are straight demands for a mixed-
mode damage law, while robustness in the XFEM framework requires initially rigid behavior. Straightforward implementation of an initially rigid mixed-mode cohesive law results in a singularity for zero opening and zero opening (see Figure 4) which harms computational stability. Two strategies are devised to remove this singularity from the cohesive [2,5].

Fiber failure can then still be modeled with continuum model [4], although the question remains how to deal with the statistical strength distribution that significantly affects the fiber failure process in some cases.

**LAMINATE FAILURE**

For analysis of a laminate a representation of delamination needs to be with the model for the elementary ply. For this purpose, interface elements are the method of choice, since they can be placed easily between the layers of solid elements that represent the different plies. A mixed mode damage law is applied which takes into account the dependence of fracture toughness on the mode ratio.

Since XFEM is used in the solid elements, information about cracks should be transferred to the interface elements. However, it is shown that this can be ignored without significant loss of accuracy under two conditions [3]. Firstly, the phantom node version of XFEM must be used, because then the displacement of the original nodes remains the actual displacement of the corresponding material point after enrichment of the material. Secondly, a nodal integration scheme must be applied for the interface elements, such that the relative displacements are only sampled at those points where the unenriched kinematics are equal to the enriched kinematics (see Figure 5).

Furthermore, in laminate analysis matrix cracking can occur as a distributed phenomenon. And because a discrete representation of matrix cracks is used, a minimum spacing must be set between those cracks. Although the chosen value for the spacing influences the crack pattern, it is shown that the exact value which is chosen for the spacing has only a small influence on simulation results such as peak load and total energy dissipation [3].

**VALIDATION**

The framework is validated through simulation of several open hole and compact tension tests [5]. In a series of experiments performed at the University of Bristol for these two test setups on the same material with different sizes and stacking sequences, size effects have been measured in the failure stress and different failure mechanisms have been observed for different configurations. These size effects are understood to be a consequence of the interaction of the different failure processes. Therefore, these tests pose a challenge for computational models. The motivation to develop reliable computational models is present in the size effect that make strength prediction challenging, while the difficulty for
building such models is present in the interaction between the different failure processes.

For the simulations, material parameters are taken from earlier simple tests performed on unidirectional plies of the same material. Because of the level of detail in the developed model and the good documentation of the experiments, it is possible to compare the predicted type of failure and amount of subcritical damage with the experimental observations (see Figures 6 and 7). And indeed the same failure mechanisms were obtained. Strength values also matched reasonably to very well in the different cases. Size effects were captured particularly well in the failure mechanisms that were dominated by delamination and matrix cracking. In fiber failure dominated cases, however, size effects were not captured so well.

**Conclusions**

The main innovation in this work has been to model matrix cracks with XFEM while enforcing the cracks to be straight as the microstructure dictates them to be in composite laminates. In an effort to embed this idea in a complete computational framework for progressive failure analysis, several issues have been encountered and tackled: initially robust mixed-mode cohesive laws, interaction between matrix cracking and delamination, transverse crack spacing, interaction between matrix cracking and fiber failure, and computational robustness and efficiency in cases with many concurrent nonlinear processes.

The thus developed model has been shown to give accurate predictions in several demanding cases. Different failure mechanisms can be represented realistically, which means that the type of failure and extent of subcritical damage can also be predicted. This is prerequisite for reliable prediction of strength and damage tolerance of composite laminates.

**References**


F.P. VAN DER MEER
Taking into Account Polydispersity for the Modeling of Liquid Fuel Injection in Internal Combustion Engines

Context

The context of the PhD is the simulation of fuel injection in an internal combustion engine, in order to improve its thermal and ecological efficiency. It more generally concerns any industrial device involving a multiphase flow made of liquid fuel injected in a chamber filled with gaz: automotive or aircraft engines, or turbo machines. In and of itself, it is possible to simulate this flow without any modeling. However the small structures created during injection (droplets of diameter until 10 μm or less) lead to a prohibitive computational cost for any industrial application. Therefore modeling is necessary. In this context, two areas are formally distinguished: the dense liquid core close to the injector called separate-phase flow, and the spray made of a polydisperse droplet population (i.e. droplets with different sizes) generated after the atomization processes downstream of the injector.

These two classes of models have each one their own research axe, with very rare connexions between the formalisms. Eventually though, a realistic fuel jet computation will need an accurate description of both the areas implying a coupling between the models.

This PhD work investigates Eulerian models for the description of polydisperse evaporating sprays, in the perspective of a further coupling for industrial computation. They represent a promising alternative to Lagrangian models, widely used at present, yet suffering from major drawbacks. Coupling a Lagrangian model to a separate phase model that can only be Eulerian, represents the major of these difficulties. Other difficulties concern its cost in unsteady configurations, while parallel computing is not natural with a Lagrangian formalism, and also the coupling with the gaseous phase, that is Eulerian.

As a first step, the Eulerian Multi-Fluid model (see [2] and references herein) has been assessed. Although it is very promising, two difficulties are highlighted: its cost for a precise description of polydispersity, and its inability to describe particle trajectory crossing (PTC). These difficulties are tackled along the Thesis. Besides, the ability to describe polydispersity is implemented in an industrial code, paving the way for industrial computations.

Modeling and Numerics

At low values of the liquid volume fraction ($\alpha < 10^{-2}$), the spray is considered a point-particle population with no interaction between each other, and can be modeled by a kinetic theory, similar to the theory for gas dynamics. This statistical approach involves a number density function (NDF) $f$ taking value in a phase space $(S, u)$ where $S$ and $u$ respectively denotes size and velocity, such as $f(t, x, S, u) dx dS du$ is the probable number of particles in the physical volume $[x, x + dx]$ and the phase...
space volume $dSdu$. This NDF is the solution of a kinetic equation, called Williams-Boltzmann equation [10]. In our study case, neither thermal effects nor collision, coalescence, fragmentation are considered, leading to the following equation:

$$\partial_t f + \nabla_u \cdot (uf) + \nabla_s \cdot (Ff) - \partial_s (RF) = 0 \quad (1)$$

where $\partial_t f + \nabla_u \cdot (uf)$ represents the free transport of the spray, $F = \partial_s (u_f)$ is the acceleration applied on droplets per unit mass (which reduces to Stokes drag in our study), $R = -\partial_s (S)$ is the evaporation term.

Given the number of dimensions of the physical and phase space, the numerical resolution of this equation is intractable. The strategy is then to reduce the phase space dimensions using moment methods, where $f$ is solved through conservation equations on some of its moments, defined by:

$$m_{ij} = \int \int \int u^i u^j f \, dsdu.$$  

This proceeds in two steps: equations on velocity moments conditioned by size are considered, making the velocity dimensions vanish, and then taking size moments of the previous equations leads to the final system of equations.

Focusing on the size distribution, there are traditionally two classes of models: sectional models and high order moment methods. The first consists in partitioning the size phase size in sections. For each section, a fluid system of equations is written considering only one size momennt (the volume), so that the precision is proportional to the number of section considered. An example of this type of model is the Multi-Fluid model [2]. But in three special dimensions, one section accounts for four transport equations, so that very few sections can be considered for computations to meet industrial timescales. The second class of model, instead of partitioning the size phase space, considers several size moments of the NDF. Although these methods are promising they are not mature enough (see [6] and references herein) to describe the evaporation flux accurately and stably. Therefore one the contribution of this Thesis has been to provide a high order moment method with stable and accurate tools for evaporation and advection of the moment vector: the EMSM model (Eulerian Multi Size Moment).

The NDF is assumed to have the following profile: $f = n(t, S) \delta(u - u_p(t, x))$ where all the particles have the same velocity $u_p$. The final system of equation contains $N$ conservation equations on the first $N$ size moments (from order 0 to $N - 1$), and one equation on the particle momentum. The key property of this model is the fact the moments are related to each other being moments of a distribution function. They belong to the so called moment space, defined and studied in the moment theory [3].

The preservation of the moment space is the big challenge when designing stable numerical tools, for evaporation and transport. The model are designed in the context of a one-way coupling, in order to assess the quality of the moment resolution. Note that the model can be extended to a two-way formalism.

To be as accurate as possible, each operator is treated separately in the context of a splitting strategy. This enables to design tools specifically suited for each operator, evaporation and transport (the drag term resolution does not bring any difficulty). The evaporation term is first considered. In the corresponding system, an unclosed term appears: $n(t, S = 0)$, a punctual value of the size distribution. Constructing a distribution from its $N$ first moments consists in solving the finite Hausdorff moment problem. Among possible solutions, an Entropy Maximization (from the information theory) is used to solve this tough problem. A closed system of time ODE is obtained, where evaporation can be decomposed of a source term accounting for the disappearing particles, and a transport term in the size phase space accounting for size decrease of existing particles. Basic explicit time integrators like Runge-Kutta schemes do not preserve the moment space and are thus unstable. Therefore, a new type of scheme has been designed, combining two tools. The source term is computed through a kinetic scheme. A kinetic scheme is a finite volume scheme relying on the kinetic level of description (using the kinetic equation) in order to compute the fluxes for moments. This type of scheme is particularly suited when the waves of the problem are explicitly known at $tn$, and enables an exact time integration of the fluxes. The transport term is solved using DQ MOM (Direct Quadrature Method of Moments). This method consists in solving directly the evolution of nodes and abscissas given by a quadrature of the NDF, which appears in this case to read easier than the evolution of the moments themselves. Details of the method are available in [9].

For the advection term, the model is closed. The difficulty is numeric since high order schemes ($order \geq 2$) lead to the corruption of some of the moment vectors. This is an know issue which has been addressed in a recent past, but with no entirely satisfactory solutions. i.e. numerous tests need to be set or additional algorithms need to be used. This potentially leads to serious increase of the computational time. Another difficulty pertains to the velocity distribution profile, introducing the pressureless gas formalism, preventing the use of any Riemann solver. Since this issue was already tackled in [2] we refer to it for related explanations. The scheme proposed in this work has the essential advantage of preserving the moment space per se [8]. Since the equations are conservative, a finite volume scheme is the natural choice. It relies on three elements. First, using the theory of canonical moment suggests quantities verifying a transport equation to be reconstructed with a simple condition for the moment space to be preserved. Then, flux computation with kinetic
schemes allows to do an exact time integration. This exact time integration is possible thanks to a dimensional splitting where equations are solved dimension per dimension.

In order to assess the EMSM models and its numerical tools, they are implemented in the MUSES3D code, an academic DNS solver that provides a framework devoted to spray method evaluation [2].

Figure 2 presents a comparison between the EMSM model solving for four size moments and the Multi-Fluid model with ten sections, on an unsteady weakly turbulent free jet configuration. Fuel gas equivalence ratio are compared. The excellent level of comparison and the fact that the Multi-Fluid model has been validated by comparisons with Lagrangian models [2] validates the EMSM model. The time efficiency is also assessed since the EMSM is four times as fast as the Multi-Fluid model. This factor should increase in three dimensions for reasons explained in [6].

Generally, Eulerian models (be it for polydisperse or monodisperse spray) account for a single velocity per droplet size. They are thus unable to describe PTC between same size droplets.

To overcome this limitation, the idea is to augment the information on the velocity distribution, increasing the number of transported moments. This is the same idea as for the EMSM model, applied to velocity moments. Since the advection flux for the $k^{th}$ moment involves the $(k + 1)^{th}$ moment, the system of equations is unclosed. The flux are determined using QMOM (Quadrature Method of Moment), a quadrature method where the fluxes are computed from the weights and abscissas given from the moments quadrature. This model is called EMVM model (Eulerian Multi Velocity Moment).

In terms of modeling, the mathematical structure of the transport system has been thoroughly studied, and has lead to fundamental results for the future design of high order schemes [1].

Although QMOM is well suited only for monovariate distribution only, in two dimensions, the distribution depends on the two components of the velocity. Nonetheless, the EMVM model has been extended to multi-dimensional configurations, based on the results of [5]. Moreover, polydispersity and PTC can be accounted for within a same model. Therefore, the EMVM model has been coupled to the Multi-Fluid model [7], and also to the EMSM model providing a formalism that overcome the two limitations of Eulerian model relative to Lagrangian models.

In terms of numerics, a finite volume scheme is considered given the conservative nature of the equations. It is first order accurate, relying on a kinetic scheme and dimensional splitting. The EMVM model coupled to the Multi-Fluid model is implemented in the MUSES3D code as well.

Figure 3 presents comparisons between the EMVM and the Multi-Fluid models. It consists in a liquid monodisperse spray cross-flow, with a Stokes number equal to 4.05, in an unsteady weakly turbulent gaseous phase. The left side of the figure present the two jets taken separately. As no collision is considered, the solution results in a pure crossing of the jet. The right side of the figure shows that the Multi-Fluid model considers unphysical collision, whereas the EMVM model is able to capture the solution.

Figure 2. Fuel equivalent ratio for evaporating sprays. Left: EMSM model. Right: Multi-Fluid model.

Figure 3. Number density for non evaporating sprays. Left: Dynamics of single sprays. Right: Dynamics of superposed sprays; top: with EMVM model; bottom: with Multi-Fluid model.
Towards industrial computations...

The last step of this work was to make the EMSM model operational to tackle industrial configurations.

The first aspect, theoretical, was to adapt it to formulations involving moving geometries, which is very common in the automotive industry because of the moving piston. A second order in time and space transport scheme for the moments has then been designed in the ALE (Arbitrary Lagrangian Eulerian) formalism [4].

The EMSM model is then implemented in the IFPC3D code, a 3D unstructured RANS reactive flow solver with spray, dedicated to internal combustion engines. This implementation has notably been validated by a comparison with a DNS computation run with the MUSES3D code. Two significant test cases are presented, that assess the new code functionality.

The first test involves a moving piston during a crank revolution perturbing a field of particles (represented by its size moments) initially uniform. Figure 4 displays results for the two first size moments at four angles. The apparition of the singularities at the piston vicinity (schematically represented in blue) is a characteristic effect of the pressureless gas dynamics. Since there is no pressure term in the momentum equation, there is no acoustic wave transmitting the density increase at the piston. Then, particles keep on accumulating until compression is over, while the field downstream of the piston stays homogeneous. During the expansion phase, the singularity keeps moving at the velocity transmitted by the piston. The signal expansion is due to numerical diffusion, but also to the expansion of the numerical cells.

Finally, the feasibility of spray injection has been proven with the type of results such as displayed in Fig. 5. It shows a comparison between the EMSM model and a Lagrangian computation, for the particle number density and velocity field. This result, qualitatively satisfying, though in a simplified configuration involving low velocity and no turbulence model, paves the way for further developments towards that direction.

REFERENCES


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Some Information about the Participation to ECCOMAS Thematic Conferences & Special Interest Conferences 2011

Most of the conferences organized in 2011 are related to "Computational Solids and Structural Mechanics". Nevertheless a number of conferences cover a wider topics and some of them are related to Computational Fluid dynamics. From the figures we have been able to get the global attendance was around 3200 with an average participation of 170. Extrapolating this information (some information is missing, some conferences have not yet taken place) the global attendance to all those 25 conferences should exceed 4000 participants. This is to say the importance and the great success of those conferences.

18th International Conference on Computer Methods in Material Science - KomPlasTech 2011
Zakopane, Poland, January 16–19
• 140 participants
• 22 countries represented

University of Trento, Italy, April 11–15
• 46 participants

Rzeszow/Sieniawa, Poland, April 27–30
• 62 participants
• 6 countries represented

CFD & Optimization Conference
Antalya, Turkey, May 23–25
• 70 participants

III International Conference on Computational Methods in Structural Dynamics and Earthquake Engineering - COMPDYN 2011
Island of Corfu, Greece, May 26–28
• 400 participants

Computational Modeling of Fracture and Failure Materials and Structures
Barcelona, Spain, June 6–8
• 293 participants
• 32 countries represented

V International Conference on Adaptive Modeling and Simulation - ADMOS 2011
Paris, France, June 6–8
• 79 participants
• 14 countries represented

Computational Analysis and Optimization - CAO2011 dedicated to Professor P. Neittaanmäki on his 60th Birthday
Jyväskylä, Finland, June 9–11
• 68 participants
• 12 countries represented

II International Conference on Computational Contact Mechanics - ICCCM 2011
Hannover, Germany, June 15–17
• 87 participants
• 22 countries represented

IV International Conference on Computational Methods for Coupled Problems in Science and Engineering - COUPLED PROBLEMS 2011
Kos Island, Greece, June 20–22
• 320 participants
• 33 countries represented

Workshop on Higher Order Finite Element and Isogeometric Methods - HOFEIM 2011
Cracow, Poland, June 27–29
• 80 participants

Second Conference on the Extended Finite Element Method - XFEM 2011
Cardiff, UK, June 29 - July 1
• 150 participants

Multibody Dynamics 2011, V Conference
Brussels, Belgium, July 4–7
• 253 participants
• 28 countries represented

Smart Structures and Materials - SMART’11
Saarbrücken, Germany, July 6–8
• 157 participants

XI International Conference on Computational Plasticity - COMPLAS XI
Barcelona, Spain, September 7–9
• 390 participants
• 40 countries represented
TCCM2011 - Trends & Challenges in Computational Mechanics, A Conference in honor of Peter Wriggers’ 60th birthday
Padua, Italy, September 12–14
• 70 participants

International Conference on Evolutionary and Deterministic Methods for Design, Optimization and Control with Applications to Industrial and Societal Problems - EUROGEN 2011
CIRA, Italian Aerospace Research Center, Italy, September 14–16

III International Conference on Mechanical Response of Composites
Leibniz Universität, Hannover, Germany, September 21–23
• 119 participants

Simulation and Modeling of Biological Flows - SIMBIO 2011
Vrije Universiteit Brussel, Brussels, Belgium, September 21–23

IV International Conference on Computational Methods in Marine Engineering
Lisbon, Portugal, September 28–30
• 116 participants
  19 countries represented

V International Conference on Textile Composites and Inflatable Membranes
Barcelona, Spain, October 5–7
• 128 participants
  25 countries represented

VIPIMAGE 2011 - III ECCOMAS Thematic Conference on Computational Vision and Medical Image Processing
Algarve, Portugal, October 12–14
• 90 participants expected

II International Conference on Particle-based Methods
Barcelona, Spain, October 26–28
• 221 participants registered so far from 35 countries

Reduced Basis, POD and PGD Model Reduction Techniques: a Breakthrough in Computational Engineering?
Ecole Normale Supérieure de Cachan, Paris, France, November 16–18

International Conference on Recent Advances in Nonlinear Models - Structural Concrete Applications - CoRA
Coimbra, Portugal, November 24–25

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The third COMPDYN 2011 took place on Corfu Island, Greece from May 25–28, 2011. The purpose of this conference series is to bring together the scientific communities of Computational Mechanics, Structural Dynamics and Earthquake Engineering in an effort to facilitate the exchange of ideas on topics of mutual interests and to serve as a platform for establishing links between research groups with complementary activities. The Technical Programme consisted of 4 Plenary lectures, 12 Semi-plenary lectures, 28 Keynote lectures, 34 Minisymposia with more than 400 presentations total. The Plenary lectures were delivered by Al. Elnashai, C. Fellipa, T.J.R. Hughes and A. Shabana, while Semi-plenary lectures were given by O. Allix, T. Burczynski, A. Combescure, F. Filippou, G. Hulbert, J. Ingham, R. Ohayon, K.C. Park, P. Steinmann, K. Tamma, W.A. Wall and Sh. Yoshimura. The proceedings of the conference are available via the ECCOMAS website: [WWW.eCCoMas.org](http://WWW.eCCoMas.org) and will soon be indexed in SCOPUS database. The next COMDYN Conference will take place on the Island of Kos, Greece from June 12–14, 2013.
The fourth COUPLED PROBLEMS 2011 took place on the island of Kos, Greece from June 20–22, 2011. The object of COUPLED PROBLEMS 2011 was to become a forum for state-of-the-art presentations and discussions of mathematical models, numerical methods and computational techniques for solving coupled problems of multidisciplinary character in science and engineering. The goal of this conference series is to make a step forward in the formulation and solution of real life problems with a multidisciplinary nature and industrial interest, accounting for all the complex couplings involved in the physical description of the problem. The Technical Programme consisted of 11 Plenary lectures, 15 Invited sessions with 290 presentations in total. The Plenary lectures were delivered by R. Codina, L. Demkowicz, T.J.R. Hughes, S. Idelsohn, G. Karniadakis, L. Laloui, W.K. Liu, R. Ohayon, K.C. Park, T. Tezduyar and W. Wall. The proceedings of the conference are available via the ECCOMAS website: www.eccomas.org. The next conference COUPLED PROBLEMS 2013 will take place in Ibiza, Spain from June 17–19, 2013 and will be dedicated to Eugenio Oñate on the occasion of his 60th birthday.
The XI International Conference on Computational Plasticity (COMPLAS XI) was held in Barcelona on 7–9 September, 2011. The first ten conferences in the series were also held in Barcelona; in April 1987, September 1989, April 1992, April 1995, March 1997, September 2000, April 2003, September 2005, September 2007 and September 2009. The continuing importance of this research topic is demonstrated by the fact that the number of papers presented has increased from just over 100 papers in the first conference to over 330 papers at COMPLAS XI. Some 400 delegates coming from 44 different countries attended the Conference.

The developments that have taken place in the field of computational plasticity are illustrated by the contents of the papers presented at the conference. A stronger interaction between the phenomenological and micromechanical modeling of nonlinear material behavior is apparent. The development of efficient and accurate computational methods continues to be a challenging goal, while it is interesting to note the permanence of element modelling as a research issue. The blending of classical FEM with new particle-based and discrete element methods appears as a prominent area of research. Industrial forming processes, geo-mechanics, biomechanics, steel, concrete, masonry and composite structures form the core of the applications of the different numerical methods presented.


In addition, 18 Invited Sessions were organized by distinguished scientists on relevant topics of Computational Plasticity.

The conference programme can be visited at HTTP://CONGRESS.CIMNE.COM/COMPLAS2011/Frontal/ProgIntro.asp

From the feedback received we feel that the conference was a success and a landmark in the history of the
Between June 30 to July 1, 2011 the first ECCOMAS PhD Olympiad took place in Athens in conjunction with the 7th International Congress of the Greek Association for Computational Mechanics (GRACM). The ECCOMAS PhD Olympiads take place annually in different locations. The purpose of the ECCOMAS PhD Olympiads is to present the best PhD Theses approved by a University or Research Organization in Europe during the previous year and to act as a forum for exchanging new ideas, disseminating recent developments in the fields of ECCOMAS and sharing common research interests among young investigators. Every affiliated National or Regional Association to ECCOMAS is represented by a number of selected PhDs submitted for consideration for the two ECCOMAS PhD Awards. In the first ECCOMAS PhD Olympiad participated 28 young investigators from 14 different Associations. The following associations participated: ACME (UK), AIMETA (Italy), APMTAC (Portugal), CEACM (Central Europe), CSMA (France), GAMM (Germany), GRACM (Greece), ISSEC (Ireland), NCTAM/BNCM (Belgium), NMC (Nederlands), PACM (Poland), SEMA (Spain), SEMNI (Spain) and SWICCOMAS (Swiss).

In particular the following participants presented their work in Athens: Patrick Farrell and Xiaoying Zhuang from ACME (UK), Michele Conti and Massimiliano Cremonesi from AIMETA (Italy), Jorge American Oliveira Pinto Belinha, Daniel Antonio Semblano Gouveia Dias-da-Costa and Joao Filipe de Almeida Milho from APMTAC (Portugal), Tomislav Jarak and Stephan Kugler from CEACM (Central Europe), Cedric Bellis, Emilien Pierres and Thago Ritto CSMA (France), Benjamin Klusemann, Christian F. Kirches and Marco Schwarze from GAMM (Germany), Georgios Bikakis and Fotios Karoulanis from GRACM (Greece), John Healy from ISSEC (Ireland), Bert Van Genechten from NCTAM/BNCM (Belgium), Frans van der Meer from NMC (Nederlands), Zbigniew Bulinski, Adam Klimanek and Lukasz Przykowski from PACM (Poland), Carmen Rodrigo and Juan Ruiz from SEMA (Spain), Pavel Ryzhakov and Lindaura Steffens from SEMNI (Spain), Sarah Levy from SWICCOMAS (Swiss).
IACMM – ISRAEL ASSOCIATION FOR COMPUTATIONAL METHODS IN MECHANICS
A MEMBER OF ECCOMAS

ANNOUNCEMENT AND CALL FOR PAPERS

The 31st Israel Symposium on Computational Mechanics (ISCM31) will take place in the Department of Mechanical Engineering, Ben Gurion University, Bershaba, on October 21st 2011.

The scientific committee is composed of Z. Yossibah (BGU), J. Bortman (BGU) and D. Givoli (Technion).

Keynote lecturer will be Prof. Jacobo Bielak – Dept. of Civil & Environmental, Carnegie-Mellon University.

Presentations related to Computational Mechanics in the largest meaning are welcome. Abstract of submission should be sent to both zohary@bgu.ac.il and jacbort@bgu.ac.il.

One of the lecturers will be selected to and supported for the ECCOMAS 2012 conference in Vienna.

More on our site HTTP://WWW.IACMM.ORG.IL

ACTIVITY OF THE SERBIAN SOCIETY FOR COMPUTATIONAL MECHANICS IN 2011

Activity of the Serbian Society for Computational Mechanics in 2011 can be summarized in the following.

2. Participation in organizing, together with the Serbian Academy of Sciences and Arts, scientific conference "Biomedical Engineering for Human Health”, 24–25 October 2011.

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ECCOMAS 2012
EUROPEAN CONGRESS ON COMPUTATIONAL METHODS IN APPLIED SCIENCES AND ENGINEERING

VIENNA, AUSTRIA | SEPTEMBER 10–14, 2012

VIENNA UNIVERSITY OF TECHNOLOGY

INSTITUTE FOR MECHANICS OF MATERIALS AND STRUCTURES
INSTITUTE OF LIGHTWEIGHT DESIGN AND STRUCTURAL BIOMECHANICS

IMPORTANT DATES

- Mini-symposia proposal, deadline: September 15, 2011
- Mini-symposia acceptance, deadline: October 31, 2011
- Abstract submission, deadline: December 15, 2011
- Notification of acceptance: March 15, 2012
- Full-paper submission, deadline: May 30, 2012
- Early registration, deadline: May 30, 2012