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**ECCOMAS Newsletter — July 2014**

**Editors**

**Ekkehard Ramm**

Universität Stuttgart
President of ECCOMAS

**Manolis Papadrakakis**

National Technical University of Athens
Past President of ECCOMAS

**Josef Eberhardsteiner**

Vienna University of Technology
Secretary of ECCOMAS

**Ferdinando Auricchio**

University of Pavia
Vice President of ECCOMAS

**Pedro Diez**

Universitat Politècnica de Catalunya
Vice President of ECCOMAS

**Panagiota Kouniaki**

National Technical University of Athens
Technical Editor
In June 2013 the new Executive Council (EC) of ECCOMAS has been elected for a period of four years. One of the first decisions of the EC was the reactivation of the ECCOMAS Newsletter, starting with the present issue.

CONFERENCE STRUCTURE

Due to the effective previous administration, headed by President Manolis Papadrakakis, we could encounter a “warm start”. We can recognize that ECCOMAS has a very successful conference structure, see Table: ECCOMAS Congress and Conferences on Computational Solid and Structural Mechanics (ECCM) and Computational Fluid Dynamics (ECFD), alternating in even years, as well as the Thematic Conferences in odd years, when also the Young Investigator Conference (YIC) is taking place. These are supplemented by the yearly Olympiads for distinguished PhD theses awarded by the member associations. Although the Thematic Conferences (TC) were originally intended to be small state-of-the-art meetings focused on a specific topic several of them developed into medium size conferences with up to several hundred delegates. Thus this format of TCs turned out to be very flexible and successful; see the list with TCs in 2015 in this issue.

Some other meetings not fitting into this structure have been added as Special Interest or Regional Conferences; for example it is expected that intercontinental Thematic Conferences in cooperation with associations in other continents will be organized.

STRENGTHENING OF ORGANIZATION

The Executive Council took actions for restructuring the management of ECCOMAS. As an example for this process it is suggested to strengthen the role and the tasks of the four Technical Committees for Computational Applied Mathematics, Fluid Dynamics and Solid and Structural Mechanics as well as for Scientific Computing. This means that they will be much more involved in the planning, organization and decisions. Every Newsletter will contain a technical article of each Technical Committee.

As the name of the Association expresses ECCOMAS is related to Applied Sciences. It could however be recognized that the main activities were related towards subjects of Solids and Structures and Fluid Dynamics; see the two main conferences. Following the objectives defined in the bylaws ECCOMAS needs more activities in other applied sciences, like applied mathematics, computational physics and chemistry, scientific computing etc.

An important second activity is the reactivation of the ECCOMAS Young Investigator Committee (EYIC); they will not only be involved in the organization of the Young Investigator Conferences and the Olympiads, but will be active in several aspects of particular interests of young scientists, see the Young Investigator Corner in this issue.

Following the proposal of the EC the Managing Board (MB) decided to establish an Award Committee operating independently of the MB.
The 2014 Medals and Young Investigator Awards have already been elected by this Committee.

It should be mentioned that the ECCOMAS webpage www.eccomas.org has been recently updated with the most actual information; we hope that this process can be perpetuated. This needs the continuous help of the member organizations and their personal members.

Several other actions will be taken in the next time, such as setting up rules for conferences and the selection of plenary and semi-plenary lecturers, the establishment of advanced schools and courses promoting the educational aspect, the cooperation with other scientific associations, stimulating the interaction between ECCOMAS and industry, just to mention but a few.

**TOP-DOWN AND BOTTOM-UP**

The members of ECCOMAS are national and regional associations. All of them are represented in the General Assembly (GA) and the Managing Board; it is apparent that the management up to now follows in principle a top-down procedure, i.e. the decisions, made by the boards, are communicated to the member organizations. The disadvantage is that the individual personal members rely on the transport of information from their association. It seems that this information line does not function in all cases. In the extreme case the personal members do not even know that they are part of ECCOMAS. How can this situation be improved? The first measure is of course that all important information on ECCOMAS and its activities is automatically transferred to the individual members. The second aspect is that ECCOMAS needs also bottom-up activities with information and proposals from the associations and their personal members.

**APPLIED SCIENCES**

John H. Argyris saying “The Computer shapes the theory” (Lecture Royal Aeronautical Society, UK, 1965) defined already a landmark in the development of Computational Sciences. At that time the notion of Computational Mechanics was coined indicating that it was an extra column besides Applied and Experimental Mechanics. In addition the restriction to Mechanics could be attributed to the fact that initially the new computational tools, in particular the Finite Element Method, were developed in this area. As often in history traditional names justifiably kept their inertia and are used even if the fields were substantially enlarged. This is certainly true for Computational
Mechanics. Associations and conferences are still attributed to this notion although their spectrum has been enormously extended, see for example our international partner, the International Association for Computational Mechanics (IACM) with its WCCM Conferences.

In the meantime other notions appeared on the market, for example Simulation-Based Engineering Science (Blue Ribbon Panel of US-NSF) or slightly modified to Simulation-Based Engineering and Science (World Technology Education Center, Baltimore, USA). Sometimes the expression Computational Engineering Science is used, often stressing rather Applied Mathematics and Scientific Computing than Engineering and Science.

ECCOMAS has made a wise decision already when it was founded in 1993: Computational Methods in Applied Sciences, following the European understanding of Engineering being also an Applied Science and anticipating the diffusion of modeling and simulation into almost all sciences.

UPCOMING EVENTS

The joint conferences of IACM and ECCOMAS on 20-25 July 2014 in Barcelona, Spain, namely the 11th World Congress on Computational Mechanics (WCCM XI), the 5th European Conference on Computational Mechanics (ECCM V) and the 6th European Conference on Computational Fluid Dynamics (ECFD VI), will be the worldwide largest meeting of our community ever. It shows the enormous impact the Computational Methods in Applied Sciences have in the meantime which is a political message, hopefully also recognized by the European Union. It is a great challenge for the organizers, the Spanish Association for Numerical Methods in Engineering (SEMNI) and the International Center for Numerical Methods in Engineering (CIMNE) at the Universitat Politècnica de Catalunya (Barcelona Tech). ECCOMAS would like to thank the three chairmen of the Conference, Professors Eugenio Oñate, Antonio Huerta and Xavier Oliver, as well as the General Manager Cristina Forace, representative for the entire organizing team, for their enormous effort in this challenging and extraordinary undertaking.

2015 will be the year for the Thematic conferences and the Young Investigator Conference (YIC); the ECCOMAS Congress is taking place in Crete, Greece, on 5-10 June 2016, see also the rear page of this Newsletter.

THANKS

I would like to thank the members of the Executive Committee as well as the chairmen of the Technical Committees very much for their constructive input; the intensive cooperation with the Secretary Josef Eberhardsteiner, Vienna University of Technology, and Iztok Potokar from the ECCOMAS Secretariat in Barcelona is a great help. I am also grateful to all who have contributed to this newsletter, in particular Professor Manolis Papadrakakis and his team for taking over the production of this issue.

EKKEHARD RAMM
PRESIDENT OF ECCOMAS
RAMM@IBB.UNI-STUTTGART.DE
ECCOMAS

Award for Best PhD Theses 2013

Since 2002 ECCOMAS confers every year the PhD Award for the best thesis in the field of Computational Methods in Applied Sciences. Since 2006 two prizes have been awarded following a thorough selection procedure.

Every person who has presented a thesis within the ECCOMAS fields of interest and was approved by a University or a Research Organization in Europe qualifies for the Award and can submit an application. Each local ECCOMAS Member Association selects one candidate thesis according to an internally decided selection procedure. The local ECCOMAS Associations send the theses to the ECCOMAS Secretariat in Barcelona where the ECCOMAS PhD Awards Committee selects two Awardees.

The meeting of the Evaluation Committee for the ECCOMAS award for the best PhD theses 2013 was held on May 9th, 2014 at CIMNE, Barcelona. As a response to the call for tender, the ECCOMAS Member Associations nominated 16 theses. The Evaluation Committee was composed by Nils-Erik Wiberg (Gothenburg; Sweden), initiator of the award and chairman, Marino Arroyo (Barcelona, Spain), Chris Lacor (Brussels, Belgium), Simona Perotto (Milano, Italy), and Josef Eberhardsteiner (Vienna, Austria), secretary of ECCOMAS.

After a detailed discussion and an extensive voting procedure the winners have been selected. The two awardees are:

Henning Sauerland

(Aachen, Germany) for the thesis "An XFEM based sharp interface approach for two-phase and free-surface flows".

Henning Sauerland studied Computational Engineering Science at RWTH Aachen University with an emphasis in fluid mechanics and combustion. He graduated in 2008 as “Diplomingenieur” joining the Chair for Computational Analysis of Technical Systems (CATS) in Aachen as Research Associate where he also made his PhD. His advisors are Professors Marek Behr and Thomas-Peter Fries. Currently he is a Postdoc at CATS, RWTH Aachen University.

Abstract of Thesis:
The aim of the thesis is the development of a flexible and accurate numerical approach for the simulation of industrially relevant three-dimensional two-phase and free-surface flow problems. Herein, the extended finite element method (XFEM) is applied in order to accurately account for discontinuities in the pressure field across the phase interface without requiring that the mesh aligns with the interface. Additionally, an adaptive mesh refinement approach is applied in the vicinity of the interface. The robustness and accuracy of the proposed approach is systematically investigated for different enrichment schemes and time-integration schemes. Yet, the XFEM is often prone to ill-conditioning of the global system matrix. Approximation properties and iterative solver performance are systematically compared for different approaches which should improve the conditioning. Finally, the XFEM two-phase flow solver is applied to three-dimensional dam breaking problems, rising droplet simulations and the complex flow in a spillway.

http://www.cats.rwth-aachen.de/Members/sauerland/Sauerland2013
Francesc Verdugo (Barcelona, Spain) for the thesis "Error assessment and adaptivity for structural transient dynamics".

Francesc Verdugo got his BSc and MsSc in Civil Engineering and graduated from Universitat Politècnica de Catalunya (UPC)-BarcelonaTech in 2009. He obtained his PhD in Applied Mathematics during his work at Laboratori de Càlcul Numèric (LaCàN) of UPC. His PhD Advisors are Professor Pedro Díez and Dr. Núria Parés. Currently he has a research position as Postdoc at the Institute for Computational Mechanics, TU München.

Abstract of thesis:
The finite element method is a valuable tool for simulating complex physical phenomena. However, any finite element approximation has two main error sources: the modeling error and the discretization error. Consequently, both errors have to be controlled to provide a reliable numerical solution. This is particularly important if sensitive decisions are taken on the basis of numerical results. This thesis aims at assessing the discretization error in structural transient dynamics. In this context, controlling the error is particularly relevant because, as compared to standard elliptic problems, the discretization errors are generated and propagated less intuitively or predictively. Nowadays, the error assessment techniques are well established for steady-state linear elasticity and other elliptic problems. However, the direct extension of these techniques to structural transient dynamics presents both theoretical and practical challenges. The present thesis proposes new error estimates for structural transient dynamics addressing the following difficulties: 1) the poor quality of the computable error bounds, 2) the cost of computing goal-oriented error estimates, and 3) the limitation of standard quantities of interest when dealing with time-dependent problems.


Both theses are outstanding works in Computational Methods combining excellent knowledge of both theory and practice. The award decision was based on the originality of the theses, its scientific contents and the innovative numerical developments.

On behalf of ECCOMAS I would like to congratulate both awardees for this excellent achievement.

Ekkehard Ramm
President of ECCOMAS
RAMM@IBB.UNI-STUTTGART.DE
In the last decade, many innovative modeling or solution techniques have been introduced in the field of computational mechanics. These techniques, such as enriched finite elements or multiscale modeling, enable performing complex simulations that are out of reach of conventional finite element analysis (FEA) tools, in terms of computational or human costs. Although these techniques have proved their performance by extensive testing on academic applications, they are scarcely applied on actual industrial problems because they cannot be conveniently implemented into commercial FEA software packages. Therefore a scientific and practical challenge is to allow realistic simulation of complex industrial problems including all their physical and technological complexity. A view on this issue can be found in a prospective document of the NSF blue-ribbon panel [1].

"If an industry is to replace testing with simulation, the simulation tools must undergo robust verification and validation procedures for effectiveness. Overall, simulation in industry has yet to meet its full potential. The following list is a summary of its current limitations:

1. The development of models is very time consuming, particularly for geometries of complex engineering systems...
2. Methods are needed for linking models at various scales and simulating multi-physics phenomena."

The proposed path consists in the development of a new class of general methods, the non-intrusive ones. The aim is, by an easy and fast coupling, to merge research software, with their enhanced physical capabilities, with industrial ones, with their geometrical and technological capabilities. The non-intrusive prerequisite is to not exert oneself modifying the industrial models and closed software whose development and maintenance require tens of specialized engineers. Another possible outcome concerns the validation of the model itself, the quality of advanced models being rarely checked on complex applications, another reason why engineers do not use the new generation of multi-scale models.

The prerequisite of the proposed non-intrusive framework is to keep unchanged the global numerical model as well as the solver used for its treatment. Therefore two or several models are used concurrently, the untouched global model and locals ones which are iteratively substituted where needed. The exchanges between the two models are such that the data should be "natural" ones for the global model such as prescribed forces. Possible applications are numerous even though the approach has to be adapted depending on the context. Some first examples mainly coming from a French National project ICARE funded by the ANR (French National Research agency) are used here to illustrate the versatility of the method for:

- local adaptation of a Finite Element model with introduction of topologi-

Figure 1. Basic sketch of the method.

Figure 2. 3D case: evolution of the error with and without acceleration: Dashed line: error at the interface, full line on the maximum equivalent plastic strain.
cal and material refinement,
- non-intrusive implementation of the XFEM method,
- local 3D refinement of a plate model with connectors,
- local treatment of stochastic models.

THE NON-INTRUSIVE PATH

The non-intrusive constraint led us to leave both the industrial mesh and solver untouched. This forbids the splitting of the mesh. A difficulty is that it is then not possible to perform computation on the complementary part of the local area, the model and mesh of this area being not available. Therefore all has to be done only by means of a separated local model analyzed with its own dedicated solver. This constraint, in turns, leads to the desirable flexibility; the local analysis being fully independent of the global one, it may be based on innovative models and numerical techniques. This implies to input only classical data to the commercial software, namely forces and displacements, a script being used to drive the corresponding global analyses. These prerequisites led us [3] to "discover" the "Iterative Global-Local" method proposed by Whitcomb [2]. Nevertheless, adaptations, discussed later, were proposed to improve the efficiency of the method [3].

Figure 1 illustrates the basic principle of the method. It is important to note that all the resolutions made on the global model (b) are elastic and performed on the unmodified mesh using the initial stiffness matrix. The method performs identically as the IGL one and quite a number of iterations are needed to achieve convergence.

NON-INTRUSIVE ACCELERATION METHOD

One reason for the possible high number of local – global iterations is the use (for the global model) of the elastic operator as in a modified Newton method. To improve the convergence rate the tangent global operator can be approximated using a symmetric quasi Newton approach of rank 1 (SR1) which is easy to implement in a non-intrusive manner by making use of the Sherman-Morisson formulae.

Another improvement can be achieved by seeking better interfacial conditions than prescribed displacements, namely mixed conditions (Robin type). The ideal interface operator is the Schur complement of the complement part but its evaluation is much too costly. Making use of ideas coming from works on the St-Venant Principle [4], this operator can be seen as containing two separated contributions. A localized one, which can be approximated by using some additional rows of elements and a large-scale contribution associated to the Saint-Venant Solution which involves in 3D six elastic computations [5]. Using such mixed conditions leads in case of localized non-linearity to very precise solutions with one or two iterations (Figure 3).

NON-INTRUSIVE IMPLEMENTATION OF THE XFEM METHOD

The question of the inclusion of a crack and its propagation in a finite element model initially not expected for this is a question that is still today the subject of numerous studies. The extended finite element method (XFEM [6]) was originally developed to overcome the high intrusiveness of remeshing based methods that may have meshing constraints near the singularity at the crack front [7]. XFEM can account for the displacement discontinuity across the crack faces, and also the tip singularity, by adding analytical enrichment functions to the classical finite element approximation subspace. It is then possible to model a crack with a mesh that does not conform to it. For crack growth simulation, conform remeshing is also no longer required at each propagation step. In this sense, X-FEM has achieved a first step towards clearly less intrusive simulation of fracture problems. Nevertheless, in industrial applications, it may happen that the initial CAD mesh is such that there are more than one order of magnitude between the scale of the structure and the size of the crack. In this case, even with the introduction of singular and

Figure 3. Local plastic strain distribution: Left: primal version (iteration 1), center: reference, right: mixed version (iteration 1)

Figure 4. Nested models (FEM, XFEM, Analytical)
discontinuous enrichments, the initial mesh may not be fine enough to simulate accurately the presence of the crack [8]. In this context the non-intrusive coupling ([2], [3], [9]) provides an effective way to make both remeshing and enrichment tasks more flexible and simple to implement and to use because the global model is left unchanged. In the case of a global linear elastic model, that means the global stiffness matrix (i.e. its factorization) and associated solver are kept unchanged when the crack grows. Efforts then focus, at the scale of the crack, on an optimally suited local X-FEM model. A localized multigrid solver (LMG) is then set up to perform the local/global non-intrusive coupling [10].

Indeed, multigrid methods [11], [12] are particularly well suited for multiscale problems, for which one can easily dissociate the short-varying part of the solution (singular crack tip displacement) from the long-varying part (coarse global displacement).

Here, the LMG is used for solving large-scale problems by splitting the scales with appropriate models and refinements. A model involving only standard finite elements is employed over the whole global domain, which plays the role of the coarser grid. An adaptive X-FEM based model is then introduced over the evolving localized domain, the finer grid, to describe the crack propagation.

One important feature of multigrid methods is that they are ready for nested models, and therefore, the local model itself can be enriched by another local patch. For instance, most propagation laws are based on stress intensity factors, that classical X-FEM is not able to provide directly. Other tip enrichments exists that directly provide reliable SIF estimates [13], [14]. Starting from a classical X-FEM formulation, this special tip enrichment can be made non-intrusive by its coupling with an analytical patch at the vicinity of the crack tip. A model can thus be constructed by the coupling of three nested models: FEM at the scale of the structure, X-FEM at the scale of the crack, Analytical at the scale of the crack tip singularity (Figure 4).

LOCAL 3D REFINEMENT OF A PLATE MODEL WITH CONNECTORS

Many industrial parts are described as an assembly of plates and shells models that are inaccurate around edges and connectors. To enrich those models by local 3D analysis and to rely on the non-intrusive framework [3], the idea followed in [15] is to build 3D Finite Element recovery of the stresses and displacements throughout the thickness of the plate thanks to the resolution of 8 3D Finite Element problem associated to unitary plate loading. This recovery depends only of the stacking sequence. For a primal version, warping vectors (Figure 7), weighted by the generalized force components of the plate solution, are used to enrich the plate displacements.

![Figure 5. Cracked three-point bending plate (Global model and local cracked patch)](image1)

![Figure 6. Locally cracked planetary carrier](image2)

![Figure 7. Wrapping vectors in case of an isotropic plate (a) and for a [0°, 90°]s laminate (b) associated to a unitary plate shear loading of the cell](image3)
The 3D model introduces a refined modeling of the bolt as well as contact and is computed using COFAST [16] dedicated software developed at LMT. The initial plate solution is therefore quite wrong but the iterative non-intrusive process allows correcting the solution quite efficiently.

The interest is then to be able to rely on tools previously developed for model of same dimension and to avoid spurious edge effects at the interface between the 2D and 3D models.

An example of the analysis of two bolded plates submitted to tension first analyzed with a crude model of an assembly of plates with a connector that does not take the coupling between tension and flexion into account where the contact between the plates is neglected is presented figure 8.

**LOCAL TREATMENT OF STOCHASTIC MODELS**

A challenging issue concerns the propagation of uncertainties in complex multiscale models.

The method proposed in [18] takes advantage of the localized side of uncertainties (see figure 9a). It relies on a global-local iterative algorithm that requires the successive solution of simple global problems (with deterministic operator) defined over a deterministic domain and of stochastic local problems (with uncertain operator, source terms or geometry) defined over patches of interest (see Figure 9b). The multiscale coupling approach appears to be flexible and non-intrusive as it allows considering different independent global and local models and solvers. Stochastic local problems can be solved using sampling-based approaches, with adaptive sampling techniques allowing the control of the accuracy of local solutions. Sampling-based approaches only require evaluations of the solution of local deterministic models that can be efficiently performed in parallel and using standard deterministic solvers, therefore preserving the non-intrusive character of the multiscale coupling strategy.

The local treatment of uncertainties allows reducing the complexity of the representation of the random solution, represented as a global solution (with low spectral content) substituted by local solutions defined on the patches (see Figure 10 for an illustration on a thermal diffusion problem).

**CONCLUSIONS**

The versatility of the method should allow to deal with a large variety of problems and for example to drastically simplify the introduction of multi-scale computation within existing industrial software as done with Abaqus and code-ASTER used in the previous examples. The method was also used and adapted to the coupling of 3D meso-model of composites and hybrid discrete continuous damage model in [16]. Other approaches have been proposed in the literature as in [9] where a non-intrusive approach based on the property of the Partition of Unity was used.

The method can also be adapted to the multiscale time-space analysis of structures in explicit dynamics [17].
REFERENCES


15. Champaney, L: Cognard, JY; Ladevèze, P., Modular analysis of assemblages of three-dimensional structures with unilateral contact conditions Computer & Structures (73:1-5) 249-266 (1999)


17. Bettinotti O ; Allix O ; Malherbe B. Coupling strategy for adaptive local refinement in space and time with a fixed global model in explicit dynamics Computational Mechanics (53:4) 561-574 (2014)


OLIVIER ALLIX, P. GOSSELET
LMT/ENS CACHAN

J-C. PASSIEUX, M. SALAUN,
M. DUVAL
INSAT DE TOULOUSE
INSTITUT CLÉMENT ADE

A. NOUY, M. CHEVREUIL
GEM/ECOLE CENTRALE NANTES

ALLIX@LMT.ENS-CACHAN.FR

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The fascination of humanity with fluid flows is ancestral. For thousands of years we have tried to understand the fluid mechanics that govern our world. The present challenges of humanity such as energy, climate change, water supply and health hinge on this understanding. Fluid flows are important for the beating heart and the metastasis of cancer as well as for the flight of airplanes and transport of pollutants. Over the last hundred years researchers have made significant theoretical, experimental and computational advances in fluid mechanics. Our generation is blessed by unprecedented technologies enabling studies that were unimaginable a decade ago. Experimental and computational "lenses" zoom from the fluid mechanics that shape galaxies, to the vortex wakes of flocking birds and the hydrophobic behavior on nanopatterned surfaces. We no longer limit ourselves to understanding fluid flows and we boldly aim to control and predict their behavior.

However along with emerging new frontiers old challenges remain. What are the fundamental mechanisms of turbulence? How to interface simulations with experiments and to exploit the unprecedented amounts of data? How to use effectively modern computer architectures? How to model flows interacting with multiple deforming bodies and biochemical phenomena across scales? We attempt some answers to these questions from the perspective of research at the Computational Science and Engineering Laboratory at ETH Zurich (www.cse-lab.ethz.ch). Our group examines fluid mechanics problems as they emerge in Engineering and Life Sciences and focus on their common computational hallmarks. We integrate Imaging, Multiscale Modeling, Uncertainty Quantification and Stochastic Optimization to study nanoscale flows, transport phenomena in cancer, fish schooling and cloud cavitation collapse.

PARTICLES AND GRIDS

What is the most effective way to simulate fluid flows? Researchers often spar over grid based or meshless/particle methods. Particles, coupled with Lagrangian descriptions of the governing Navier Stokes equations as in vortex methods and Smoothed Particle Hydrodynamics (SPH), provide automatic adaptivity and arguably require a minimal number of computational elements [7]. Grid based methods, associated with Eulerian descriptions, are known to exhibit higher accuracy. We argue that we can get the best of both worlds by coupling particle and grid based methods. In remeshed vortex methods and remeshed SPH the particles handle the convective part of the flow [12] and the representation of surfaces through Lagrangian particle level sets [8]. When the flow distorts the particle locations we map particle properties onto cartesian grids to ensure the convergence and accuracy of the method. The grid nodes become the new particles in the following iteration. This hybrid approach has several advantages. The regularity of the data structures associated with cartesian grids enables efficient solutions of the diffusion and Poisson equations. More importantly, they enable multiresolution simulations, by using wavelet adapted grids to further economize on the number of computational elements [6]. One example of such computations is shown in Figure 3, where multiresolution remeshed vortex methods are employed to study fish schooling.

Particles can be viewed as a discretization tool serving as quadrature points for the integral formulation of the Navier-Stokes equations. They also render themselves to modeling fluid systems.
by specifying interaction rules between particles. Techniques such as Molecular Dynamics, Dissipative Particle Dynamics and Discrete Element Methods are the undisputed methods of choice for simulations of nanoscale and mesoscale flow phenomena and granular systems. These particle descriptions can in turn be used to provide a unifying particle based framework bridging atomistic and continuum phenomena [9]. We devise effective algorithms for coupling particle descriptions for atomistic, mesoscale and continuum systems involving complex molecules using ideas from control theory. However several challenges remain. Remeshing is not easily extended to compressible flows and flows with discontinuities. Recent works by Cottet have elucidated a key relationship between remeshed particle methods and finite differences. This can lead to better understanding of the advantages and relations between particle and grid based methods.

**OPTIMIZATION AND UNCERTAINTY**

We focus on optimization methods that are suitable to fluid mechanics problems studied either experimentally or by expensive simulations. Bio-inspired algorithms, such as evolution strategies, are well suited to black-box optimization problems but they have a significant computational cost as they require a large number of iterations. We have developed stochastic algorithms such as the Covariance Matrix Adaptation Evolution Strategy- CMA-ES that exhibit fast convergence rates [10]. These algorithms have been applied to numerous applications, ranging from optimal fuel injection for turbine burners to reverse engineering of anguilliform swimming. In parallel, we explore stochastic algorithms to bridge data and simulations via Uncertainty Quantification and Propagation techniques (UQ+P). Our first focus has been the UQ+P of MD and DEM simulations [3]. We find that data driven approaches are essential in developing suitable interaction potentials and provide a systematic framework for predictive capabilities of particle based models.

**SURVIVAL HYDORDYNAMICS**

We have always sought inspiration from Nature to devise Engineering systems. However we may ask whether Natural creations are indeed optimal? And to what extent concepts from Nature are pertinent to Engineering devices? Can we do better?

We study such question by introducing the use of reverse engineering approaches to relating different cost functions (speed, efficiency) to swimming patterns for anguilliform swimmers. We have studied escape mechanisms on larval...
fish and found that indeed they are hydrodynamically optimal [5]. Our results have shown that fast escape speeds hinge on a remarkable balance between the momentum imparted on the fluid by the bending body of the fish and vorticity created by its tail. Our simulations have also shown that indeed we can do better than Nature if we allow for shapes and motions that may be feasible by robotic swimmers. Current work involves the simulations of schooling fish. Our results indicate that flow mediated interactions are essential components for the organization of such schools and swimmers must constantly adapt their motion to compensate for hydrodynamic interactions.

NANOSCALE FLUID MECHANICS

Nanotechnology offers the possibility of interacting with flows at the molecular scale, a characteristic of particular interest for biological systems. The difficulty of carrying out controlled experiments and obtaining detailed quantitative information on nanoscale systems makes computational studies irreplaceable. We perform large scale Molecular Dynamics Simulations of fullerenes [11], water and biomolecules interactions and we work with experimentalists and quantum chemists to assess the uncertainty in our simulations. Our simulations have questioned the superfast transport of water on carbon nanotube membranes (Figure 4) and have provided a rational explanation to such phenomena [4]. Current work focuses on flows on superhydrophobic surfaces and the transport of nanoparticles in blood capillaries as they pertain to cancer therapy.

FLUID MECHANICS OF CANCER AND ITS THERAPY

Transport phenomena are essential for the growth and metastasis of cancer [1]. Blood vessel formation due to growth factors released by tumor cells is one of the hallmarks of cancer. We have developed a computational model of this process quantifying several biological assumptions and their dynamic interactions. Blood vessels and the Extracellular Matrix are implicitly modeled using particle level sets. Current work integrates these descriptions with models of circulating tumor cells and nanoparticles. These simulation capabilities are paving the way for parallel experimental and computational studies of antiangiogenic therapies.

SUMMARY

We outline a framework for coupling particle and grid based methods for simulations of fluid mechanics problems as they emerge in Engineering and Life Sciences. Our methods rely on innovations in coupling applications with Information Technology (from Software Engineering to Machine Learning) and Mathematics (Stochastic Methods and Multiscale modeling). Looking forward I envision a closer interaction of experimental and computational efforts that goes beyond the passive exchange of data and involves their active integration for studying and controlling flow phenomena. I believe that Computational Fluid Dynamics will be making valuable contributions to our society, by helping to solve energy Problems, reduce Pollution and cure Cancer.

BIBLIOGRAPHY

NOTE: the Bibliography refers only to research performed at the CSE Lab. We acknowledge important contributions to our work from many colleagues and we refer the reader to the references of the articles listed below.


8. S. Hieber, P. Koumoutsakos, A Lagrangian Particle Level Set Method, J. of Computational Physics, 210,2005


Figure 4: MD simulations of water transport in Carbon Nanotube Membranes
INTRODUCTION

The term “Auxetic materials” is used to describe mechanical metamaterials with negative Poisson’s ratio (NPR materials). It originates from the Greek word afxetos (αυξητός), meaning something which increases. The majority of materials in nature have a positive Poisson’s ratio, meaning that when stretched in one direction, they get thinner in the other two perpendicular directions (and vice versa). The opposite effect takes place in materials with negative Poisson’s ratio. On the other hand, NPR materials behave exactly the opposite: when stretched they become thicker and vice versa. This effect is commonly attributed to the microstructure: the microstructure shown in figure 1.b leads to auxetic behavior and can be studied as a compliant mechanism.

Compliant mechanisms are monolithic, but flexible structures that transform external loading to motion. The absence of joints makes the production of compliant mechanisms in micro and nano scale possible. A very popular method, used for the design of compliant mechanisms is topology optimization. Finally, the resulting material distribution, taken from topology optimization, after possible modifications of the end-user, can be validated using numerical homogenization.

TOPOLOGY OPTIMIZATION - THE HYBRID SCHEMA

Topology optimization is formulated as an optimal material distribution problem inside a fixed design domain with reference to a specified objective function and a set of constraints [7]. The resulting structure, for a given set of loads and boundary conditions, meets a predefined set of performance goals. The topology optimization problem can be considered as a “0-1” integer optimization problem. In the beginning, the design domain is discretized into finite elements. In each finite element a design variable of density $x$ is assigned. If density is equal to one, material is present in that area and the cell is painted in black, otherwise there is no material and the cell is void. The problem can be relaxed by substitution of the integer variables with continuous ones, powered in a penalty value $p \geq 3$, leading the design variables near to the ideally desired discrete values 0 and 1. The method is called SIMP (Solid Isotropic Material with Penalization).

All iterative techniques used in structural or mechanism topology optimization are local iterative optimization methods or heuristics. Therefore, in the case of nonconvex problems, they will stop at local minima. In fact, starting from different initial material distributions leads to completely different final topologies. Therefore the need of using global optimization techniques arises. The usage of mathematical global optimization algorithms for such a large optimization problem is not suitable. Usage of evolutionary or genetic algorithms is, in principle, applicable. On the other hand, the operators used in evolutionary algorithms do not guarantee that in every step of the algorithm, one gets a realizable structure with invertible stiffness matrix. For that reason tailored operators are needed to keep structural solidity, and this makes every development case-dependent. In this case a hybrid optimization scheme is used, which is described in figure 2.

Figure 1. Positive and negative Poisson's ratio behavior of microstructures
PROBLEM DEFINITION

As an example of a compliant mechanism design problem, the Representative Volume Element shown in figure 3 is considered. The design criterion is to create a microstructure that behaves as an auxetic material [3,4], similar to a star-shaped structure [1,2], thus when a tensile load is applied to points A, A', the points B and B' are moving upwards and downwards respectively. Axisymmetric constraints can be applied to reduce the problem to one quarter.

TOWARDS COUPLING TOPOLOGY OPTIMIZATION AND HOMOGENIZATION

Let us consider the microstructure designed previously, possibly modified in order to cover manufacturability or other criteria and embedded into a weak matrix material in order to form a composite material. Its mechanical properties can be verified using numerical homogenization [5,6]. For demonstration purposes, let us use two materials: one strong material (density=1), and another soft material (with density<0.6). Linear displacements, which satisfy the Hill-Mandel energy principle, are the loading of the RVE. After solution of the linear finite element model, the average stress vector \( \mathbf{\sigma}_{vm} \) is estimated. Then, the effective elasticity tensor \( \mathbf{E}^* \) in plane stress conditions is calculated by applying \( \mathbf{\sigma}_{vm} = \mathbf{E}^* \mathbf{\epsilon}_{vm} \), where \( \mathbf{\epsilon}_{vm} = \mathbf{\epsilon}^M \) (loading strain). The results are strongly related to the initial material parameters given for the soft material. For the strong material the material properties are: \( E_{str}=1 \), \( \nu_{str}=0.1 \). The same values have been used in the topology optimization procedure, for the material with density=1. For the soft material, values equal to \( E_{soft}=0.007 \), \( \nu_{soft}=0.007 \), lead to an auxetic behavior of the RVE, with Poisson ratio equal to \( \nu_{eff,xy} = -0.2433 \), \( \nu_{eff,yx} = -0.2484 \). These values are compared well with the respective value of the Poisson ratio obtained by the topology optimization, which is equal to \(-0.223\).

RESULTS

Figure 4, presents a continuous formulation of auxetic microstructure as it is obtained by topology optimization. In figure 4d the displacement of the hard material given by the homogenization approach, is shown. According to this figure, a negative Poisson ratio arises for the structure. This effect remains visible even if the microstructure is embedded into a soft matrix material in order to form a composite medium, provided that the matrix is not strong enough.
CONCLUSIONS

A complete design procedure for the creation of novel auxetic microstructures has been presented here. The method can be extended to cover the design of metamaterials in multiphysics applications, like the design of thermoelastic microstructures with negative thermal expansion rate, in magnetoelectronics etc. Classical numerical homogenization has been used, for the validation of the results obtained by topology optimization. The auxetic behaviour, as well as the effective Poisson’s ratio have been verified. Further research may include nonlinear problems with large deformations, material nonlinearity and contact effects.

ACKNOWLEDGEMENTS

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REFERENCES


GEORGIOS STAVROULAKIS
NIKOLAOS KAMINAKIS
TECHNICAL UNIVERSITY OF CRETE
INSTITUTE OF COMPUTATIONAL
MECHANICS AND OPTIMIZATION
GREECE

GEORGIOS DROSOPOULOS
LEIBNIZ UNIVERSITY OF HANNOVER
INSTITUTE OF CONTINUUM
MECHANICS
GERMANY

GESTAVR@DPEM.TUC.GR
RATE OPTIMALITY OF ADAPTIVE ALGORITHMS

The overwhelming practical success of adaptive mesh-refinement in computational sciences and engineering has recently obtained a mathematical foundation with a theory on optimal convergence rates. This article first explains an abstract adaptive algorithm and its marking strategy. Secondly, it elucidates the concept of optimality in nonlinear approximation theory for a general audience. It thirdly outlines an abstract framework with fairly general hypotheses (A1)–(A4), which imply such an optimality result. Various comments conclude this state of the art overview.


1 THE ALGORITHM

The geometry of the domain \( \Omega \) in some boundary value problem (BVP) is often specified in numerical simulations in terms of a triangulation \( \mathcal{T} \) (also called mesh or partition) which is a set of a large but finite number of cells (also called element-domains) \( T_0, \ldots, T_N \). Based on this mesh \( \mathcal{T} \), some discrete model (e.g., finite element method (FEM)) leads to some discrete solution \( U(\mathcal{T}) \) which approximates an unknown exact solution \( u \) to the BVP. Usually, a posteriori error estimates motivate some computable error estimator

\[ \eta(\mathcal{T})^2 = \sum_{i=1}^{N} \eta_{T_i}(\mathcal{T})^2. \]

The local contributions \( \eta_{T_i}(\mathcal{T}) \) serve as refinement-indicators in the adaptive mesh-refining algorithm, where the marking is the essential decision for refinement and written as a list of \( \mathcal{M} \) cells (i.e. \( \mathcal{M} \subseteq \mathcal{T} \)) with some larger refinement-indicator. The refinement procedure then computes the smallest admissible refinement \( \mathcal{T}' \) of the mesh \( \mathcal{T} \) (see Section 3) such that at least the marked cells are refined.

The successive loops of those steps lead to the following adaptive algorithm, where the coarsest mesh \( \mathcal{T}_0 \) is an input data.

Adaptive Algorithm

Input: initial mesh \( \mathcal{T}_0 \)

Loop: for \( \ell = 0, 1, 2, \ldots \) do steps 1-4:

1. Solve: Compute discrete approximation \( U(\mathcal{T}_\ell) \).
2. Estimate: Compute refinement indicators \( \eta_{T}(\mathcal{T}_\ell) \) for all \( T \in \mathcal{T}_\ell \).
3. Mark: Choose set of cells to refine \( \mathcal{M}_\ell \subseteq \mathcal{T}_\ell \) (see Section 4 for details).
4. Refine: Generate new mesh \( \mathcal{T}_{\ell+1} \) by refinement of at least all cells in \( \mathcal{M}_\ell \) (see Section 3 for details).

Output: Meshes \( \mathcal{T}_\ell \), approximations \( U(\mathcal{T}_\ell) \), and estimators \( \eta(\mathcal{T}_\ell) \).

2 THE OPTIMALITY

Figure 1 displays a typical mesh for some adaptive 3D mesh-refinement of some L-shaped cylinder into tetrahedra with some global refinement as well as some local mesh-refinement towards the vertical edge along the re-entrant corner. The question whether this is a good mesh or not is an important issue in the mesh-design with many partially heuristic answers and approaches. We merely mention the coarsening techniques as in [Binev et al., 2004] when applied to the adaptive hp-FEM with the crucial decision about h- or p-refinement.

For the optimality analysis of the adaptive algorithm of Section 1, the
natural comparison for optimality is with respect to the estimator $\eta$. The underlying class $\mathcal{T}$ of simplicial meshes is based, e.g., on newest vertex bisection (NVB) of an initial mesh $\mathcal{T}_0$; see, e.g., [Stevenson, 2008]. Since the typical work load is proportional to (and expected at least to be monotone increasing with) the number of tetrahedra $|\mathcal{T}|$ in the admissible mesh $\mathcal{T}$, given any non-negative integer $N$ define

$$
\mathcal{T}(N) = \{ \mathcal{T} \in \mathcal{T} : |\mathcal{T}| \leq |\mathcal{T}_0| + N \}.
$$

Then, the accuracy is measured in terms of the estimator $\eta$, and the optimal value for meshes with $\leq N$ extra tetrahedra, namely

$$
\eta(\mathcal{T}(N)) = \min_{\mathcal{T} \in \mathcal{T}(N)} \eta(\mathcal{T}),
$$

is studied as a function of $N=0,1,2,...$ and may be compared with $\eta(\mathcal{T})$ of the computed solution and the number $N' = |\mathcal{T}'| - |\mathcal{T}_0'|$ of extra tetrahedra in the computed triangulation of level $\ell = 0,1,2,...$.

Figure 2 presents a schematic scenario in a log-log scale which is written explicitly near the axes. The entries $(N,\eta(\mathcal{T}(N)))$ are shown in red as a decreasing sequence for $N=0,1,2,...$ as well as the corresponding entries $(N,\eta(\mathcal{T}))$ for $\ell = 0,1,2,...$ in blue. By definition,

$$
\eta(\mathcal{T}(N)) \leq \eta(\mathcal{T})
$$

for all $\ell = 0,1,2,...$ The converse estimate is unclear and expected to fail in general. However, rate optimality of the adaptive algorithm leads to an asymptotic comparison: Suppose there exists a convergence rate $0 < \sigma < \infty$ in the sense that

$$
M = \min_{N=0,1,2,...} (N + 1)^\sigma \eta(\mathcal{T}(N)) < \infty.
$$

Then, optimality means that the adaptively computed solutions $U(\mathcal{T})$ with corresponding estimators allow for the same rate in the sense that

$$
\sup_{\ell=0,1,...} (N + 1)^\sigma \eta(\mathcal{T}) \leq C_{qop} M.
$$

The visualization in Figure 2 shows two parallel straight lines of slope $-\sigma$ in the log-log scaling. In fact, the log-transform of the above rate condition shows that

$$
\log(\eta(\mathcal{T}(N))) \leq \log(M) - \sigma \log(N + 1)
$$

for all $N=0,1,2,...$. In other words, this straight line is an upper bound of the entries of the optimal meshes with an additive constant $\log(M)$ and multiplicative factor $-\sigma$. The constant $C_{qop} < \infty$ leads to a shift of the upper bound for the computed entries. The parallel straight line with an additive constant $\log(M) + \log(C_{qop})$ (and the same slope $-\sigma$) is in fact an upper bound. Stated explicitly, rate optimality of the adaptive algorithm means that the computed values $(N,\eta(\mathcal{T}))$ will asymptotically below a curve parallel to the optimal curve $(N,\eta(\mathcal{T}))$.

The optimality results from [Binev et al., 2004] and [Stevenson, 2007] show that (under some conditions) the same rate holds for the computed value in the sense that the generic constant $C_{qop} < \infty$ depends only on $\mathcal{T}_0$ and on the optimal rate $\sigma$ as well as on the marking parameter $\theta$ from Section 4. The constants in the axioms of Section 5 below determine the quasi-optimality constant $C_{qop}$.

From the view of computational efficiency, not only the convergence rate $\sigma$ is important, but also the number of adaptive steps. An adaptive algorithm could refine only a few elements in each step and, despite converging with optimal rate, may turn out to be extremely inefficient (with respect to CPU time).

The above considerations are formalized in the following two main results, which hold under the axioms (A1)–(A4) of Section 5.

**Main Result 1:** The adaptive algorithm guarantees linear convergence in the sense of

$$
|\mathcal{T}_r| - |\mathcal{T}_0| \leq C_B \sum_{\ell=0}^{r-1} |\mathcal{M}_\ell|,
$$

for all $r = 0,1,2,...$ with some constant $0 < q < 1$.

**Main Result 2:** For some sufficiently small adaptivity parameter $\theta$ from Section 4, the adaptive algorithm is quasi-optimal in the sense that it reveals the optimal rate of convergence.

3 THE REFINEMENT

The most fundamental property of NVB are the $\gamma$-shape regularity, which ensures that the cells of the meshes do not degenerate (i.e., the interior angles are bounded below), and the $K$-mesh property, which ensures that neighbouring cells in the mesh are of comparable size. This is why refinement of a cell may enforce refinements of additional cells and hence generates more refined cells $\mathcal{T}' \mathcal{T}$ than marked cells $\mathcal{M}$. However, both properties are only implicitly necessary for the validation of the axioms of Section 5.

Since the number of refined cells is the only factor which distinguishes adaptive refinement from uniform refinement, it is important to control this overhead. To that end, the analysis builds on the closure estimate from [Binev et al., 2004]
where the constant $C_{\text{reg}} \geq 1$ depends only on $T_0$ and $T_{l+1}$, for all $j = 1, \ldots, \ell-1$, is the coarsest admissible refinement of $T_j$, where all cells $T \in M_j$ are bisected. Moreover, a cell of $T_{l+1}$ is refined into at most $C + 1$ son cells in $T_0$. Counterexamples in the literature (even 1D bisection) show that

$$|T_{l+1}| - |T_{l}| \leq C |M_{l-1}|,$$

cannot hold with some $\ell$-independent constant $C > 0$ for refinement strategies which satisfy the $K$-mesh property mentioned above.

The optimality analysis relies on the comparison of different meshes. To that end, it is important that each two meshes $T$, $T'$ which are refinements of $T_0$ have a coarsest common refinement $T \ominus T'$ in the sense that $T \ominus T'$ is a refinement of both $T$ and $T'$ and has less or equal cells than $|T| + |T'| - |T_0|$. Finally, a necessary requirement is that NVB has no blind ends. This means that for each refinement $T$ of $T_0$ and all $\varepsilon > 0$, there exists a refinement $T'$ of $T$ such that

$$||u - U(T')|| \leq \varepsilon.$$

Instead of NVB, any other mesh-refinement could be used which guarantees the aforementioned properties.

### 4 THE MARKING

In each adaptive step, the error estimator $\eta(T)$ gives a heuristic measure of the error on each cell $T \in T_l$. If the adaptive algorithm is supposed to reduce the error sufficiently fast (i.e. by a factor $0 < q < 1$ each step), it is sufficient and even necessary (see [Carstensen et al. 2014]) for a proof to apply the following Dörfler marking criterion [Dörfler, 1996] to identify the cells $M_l$ to be refined: Given some fixed adaptivity parameter $0 < \theta \leq 1$, find a set $M_l \subseteq T_l$ of (almost) minimal cardinality with

$$\theta \eta(T_l)^2 \leq \sum_{T \in M_l} \eta(T_l)^2.$$ 

The naive approach to find the set $M_l$ sorts the list of cells such that

$$\eta(T_l) \geq \cdots \geq \eta(T_l),$$

does not hold with some $\ell$-independent constant $C > 0$ for refinement strategies which satisfy the $K$-mesh property mentioned above.

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does not hold with some $\ell$-independent constant $C > 0$ for refinement strategies which satisfy the $K$-mesh property mentioned above.

Finally, a necessary requirement is that NVB has no blind ends. This means that for each refinement $T$ of $T_0$ and all $\varepsilon > 0$, there exists a refinement $T'$ of $T$ such that

$$||u - U(T')|| \leq \varepsilon.$$

Instead of NVB, any other mesh-refinement could be used which guarantees the aforementioned properties.

### 5 THE AXIOMS

If one aims at optimal asymptotic error reduction, the error estimator should satisfy the following four axioms. For simplicity, we abbreviate

$$\eta_k(T) = \sum_{T \in M_k} \eta(T)^2$$

for the error estimator on any subset $R \subseteq T$ of cells. The generic constants $0 < q_{\text{rel}} < 1$, $C_{\text{stab}}$, $C_{\text{reg}}$, $C_{\text{coars}}$, $C_{\text{rel}} \geq 1$ depend only on $T_0$.

(A1) **Stability:** For a refinement $T'$ of $T$, $T \cap T'$ denotes the non-refined cells. The difference of the corresponding error indicators should be bounded by the difference of the solutions $U(T)$ and $U(T')$ in the sense

$$\eta(T) - \eta(T') \leq C_{\text{stab}} ||U(T) - U(T')||.$$

(A2) **Reduction:** For a refinement $T'$ of $T$, $T \setminus T'$ contains the non-refined cells of $T$, whereas $T' \setminus T$ contains the newly generated cell of $T$. Each refinement of a cell reduces the mesh-width and hence should reduce the estimator in the sense

$$\eta(T')^2 \leq q_{\text{rel}} \eta(T)^2 + C_{\text{rel}} ||U(T) - U(T')||^2.$$ 

(A3) **Orthogonality:** Each iteration of the adaptive Algorithm improves the solution by adding $U(T_{l+1}) - U(T_l)$ to the existing approximation $U(T_l)$. The estimator $\eta(T_l)$ should control all subsequent steps of the adaptive Algorithm in the sense that

$$\sum_{k=0}^{\infty} ||U(T_{k+1}) - U(T_k)||^2 \leq C_{\text{rel}} \eta(T_l)^2.$$ 

(A4) **Discrete reliability:** The adaptive algorithm controls only the error estimator $\eta(T)$. Since the governing quantity for approximation quality is the error $||u - U(T)||$, the error estimator should bound the error from above in the sense that 

$$||U(T) - U(T')|| \leq C_{\text{rel}} \eta(T_l).$$

For some set $T \setminus T'$ contains the refined cells $T \setminus T'$. This discrete reliability implies

$$||u - U(T)|| \leq C_{\text{rel}} \eta(T_l).$$

### 6 THE HISTORY

The Main Results 1—2 of Section 2 are the accumulation of the following seminal results. [Dörfler, 1996] introduced the marking criterion from Section 4 and proved linear convergence of the error for some FEM for the Poisson problem up to some tolerance. [Morin et al., 2000] extended the analysis and included data approximation to prove convergence of a practical adaptive algorithm. [Binev et al., 2004] first proved convergence with optimal rates in the sense of Section 2 for the Poisson problem. However, their analysis required an additional mesh-coarsening step in the adaptive algorithm. [Stevenson, 2007] removed this coarsening step and proved convergence with optimal...
rates for the adaptive algorithm of Section 1. [Cascon et al., 2008] included standard newest vertex bisection as mesh refinement into the mathematical analysis.

Until then, only variations of FEM for the Poisson model problem with homogeneous Dirichlet boundary conditions were analyzed in the literature. Independently, [Feischl et al., 2013] and [Gantumur, 2013] developed the analysis for integral equations and proved convergence with optimal rates for standard boundary element methods (BEMs). For his contributions to [Feischl et al., 2013] and the field of adaptive BEM, Michael Karkulik won the Dr. Körper award 2013 of GAMM (Gesellschaft für Angewandte Mathematik und Mechanik). [Aurada et al., 2013] proved optimal convergence rates for FEM for the Poisson problem with general boundary conditions. Finally, [Feischl et al., 2014] concluded the theory for general second-order linear elliptic PDEs.

The recent work [Carstensen et al. 2014] collects all the mentioned seminal works in a unifying and abstract framework. The work identifies the axioms (A1)—(A4) from Section 5 and proves optimal rates for any problem that fits in the abstract setting. The latter covers the existing literature on rate optimality for conforming FEM (also the known results for nonlinear problems) and BEM as well as nonconforming and mixed FEM. With some additional (resp. relaxed) axioms, the abstract framework of [Carstensen et al., 2014] covers also inexact solvers and other error estimators (e.g., ZZ-type averaging error estimators).

Recently, the work http://arxiv.org/abs/1306.0377 proved for the 2D Poisson model problem that the (slightly extended) maximum strategy implies instance optimality: The adaptive meshes are pre-asymptotically optimal. One possible disadvantage is that linear convergence (Main Result 1) is not guaranteed and hence optimal computational complexity may be excluded.

7 The Complexity

The asymptotic optimality notion of Section 2 may be seen as a first and important step towards a most effective computation. The computational complexity involves the usage of the iterative solver in the adaptive algorithm. The above results hold under the underlying assumption that the discrete solution as well as the estimators is computed exactly, which is unrealistic once optimal solvers (e.g., multigrid or BPX pre-conditioned CG) are employed. Section 7 of [Carstensen et al., 2014] shows a way to modify the adaptive algorithm: One needs to control the termination error in terms of the estimator and to engage some perturbation of the arguments behind the analysis for exact solve.

The situation is more dramatic for nonlinear problems, which always require an iterative solution procedure. Under realistic assumptions on the practical performance of the algebraic eigensolver (with multigrid preconditioning) [Carstensen et al., 2012] showed overall optimal complexity. Figure 4 displays numerical simulations for the first eigenvalue of the Laplacian in the 3D geometry of Figure 1. This numerical evidence suggests a practical optimal complexity and won Joscha Gedicke the SIAM student paper prize 2013.

Despite the first success, the overall proof of optimal computational complexity has to combine an analysis of optimal mesh-design with an analysis of the iterative solution process, and the emerging theory is still in its infancy for many important applications.

Carsten Carstensen
DEPARTMENT OF MATHEMATICS
HUMBOLDT-UNIVERSITÄT ZU BERLIN
CC@MATH.HU-BERLIN.DE

Michael Feischl
Dirk Praetorius
INSTITUTE FOR ANALYSIS AND SCIENTIFIC COMPUTING
VIENNA UNIVERSITY OF TECHNOLOGY
ECCOMAS Young Investigators can be defined as young scientists (40 years old or younger) working in one of the ECCOMAS research fields. In the last years the number of young investigators working in computational methods in applied sciences has significantly increased. Therefore, the ECCOMAS Young Investigators Committee (EYIC) has been created in order to promote the main goals of ECCOMAS among young researchers, with special emphasis in encouraging activities of young ECCOMAS members. The EYIC is composed by members of each national and regional association and has a term of four years. The main tasks of the EYIC include the creation of a database of young investigators with “networking” aims (such as, for example, sharing info on research topics around Europe; sharing info on open positions; sharing info on available awards/opportunities for young people; sharing info on conferences/summer schools), to promote and facilitate the creation of “young” sections within national associations; to promote the participation of young people to ECCOMAS initiatives/conferences, etc. The EYIC convenes at least once (but preferably twice) a year, generally in correspondence of ECCOMAS events.

The next meeting of the EYIC will take place in July 2014 in Barcelona during the WCCM/ECCM/ECFD Conference.

A dedicated section of the ECCOMAS webpage is set-up in order to collect all information and announcements related to the EYIC activities.

The EYIC is currently composed by:

- ACME: William Coombs (University of Durham)
- AIMETA/GIMC: Alessandro Reali (University of Pavia)
- APMTAC: A. Andrade-Campos (University of Aveiro)
- CEACM: Eduard Marenić
- CSMA: Ludovic Chamoin (ENS Cachan)
- GACM: Alexander Popp
- GAMM: Stefanie Elgeti and Jaan-Willem Simon (RWTH Aachen), Chairpersons of YIC 2015
- GAMNI: Boniface Nkonga (University of Nice Sophia-Antipolis)
- GRACM: George Tsiatas (National Technical University of Athens)
- IACMM: Mahmood Jabareen (Technion, Haifa)
- NOACM: Fredrik Larsson (Chalmers University of Technology)
- NMC: Frans van der Meer
- ONIV: Andrey Gorobets (Keldysh Institute of Applied Mathematics)
- PACM: Piotr Siericki (Poznan University of Technology)
- SeMA: Hector Gomez (University of A Coruna)
- SEMNi: Joan Baiges (CIMNE)
- SIMAI: Lourenco Beirao da Veiga (University of Milan)
- SSCM: Miljan Milosevic (University of Kragujevac)

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After a first edition in Aveiro in 2012, the second ECCOMAS Young Investigators Conference (YIC2013) took place in Bordeaux from 2 to 6 September 2013. YIC2013 gathered about 120 participants, coming from all over Europe, in the Haut-Carré domain (an old monastery) located on the University of Bordeaux 1 campus. Ludovic Chamoin and Cécile Dobrzynski were the conference chairpersons.

The schedule of the conference was organized on five days, each one starting with a plenary session:

- the talk of G. Bal (Columbia University, USA) on Monday was on \textit{Equations with random coefficients and theories of random fluctuations};
- the talk of N. Autrusson (Safran, France) on Tuesday was on \textit{High performance computing and long term simulation challenges for air transport};
- the talk of T. Magin (Von Karman Institute, Belgium) on Wednesday was on \textit{Simulation of the material response of ablators in atmospheric entry flows};
- the talk of P. Massin (EDF, France) on Thursday was on \textit{The need for computational mechanics at EDF};
- the talk of M. Arroyo (UPC, Spain) on Friday was on \textit{Small scale Mechanics with a focus on carbon nanostructures and biomolecules}.

YIC2013 was characterized by the introduction of new creative and innovative formats adapted to the young attendance: (i) most of mini-symposia were introduced by a 30min overview talk given by a junior scientist working in the field, in order to facilitate understanding of other talks by all attendees; (ii) some plenary talks had a unusual format with the presence of an opponent whose objective was, in a theatrical way, to question the speaker and highlight scientific issues in order to increase the clarity of the presentation. Specific sessions were also introduced such as a \textit{software session} on Wednesday, and a \textit{lightning talks session} on Monday (before the welcome cocktail) with very short presentations that aimed at introducing scientific problems or ongoing works to be discussed between participants.

The YIC2013 conference also hosted the 3rd ECCOMAS PhD Olympiad and a specific session was dedicated to presentations by the two 2012 ECCOMAS PhD Awardees. A social program was proposed to YIC2013 participants and was much appreciated: a 2 hour guided walking tour of the historic center of Bordeaux (listed as a UNESCO World Heritage Site) followed by the banquet (buffet & wine cocktail) at the Grand Theatre of Bordeaux.

ECCOMAS, local associations CSMA and SMAI, as well as the numerous sponsors (Inria, EDF, Safran, EADS, AFM, CEA, Univ Bordeaux 1, IPB, Région Aquitaine, CUB) have supported this successful conference with very reasonable conference fees (150€).
We would like to invite you to join us for the YIC GACM 2015: July 20-23, 2015 in Aachen, Germany.

This Young Investigators Conference (YIC) will be the third meeting of its kind organized as ECCOMAS Conference (European Community of Computational Methods in Applied Sciences). On this particular occasion, we have the opportunity to hold the conference in conjunction with the GACM (German Association of Computational Mechanics) Colloquium for Young Scientists. As a new series of scientific events, the YIC focuses on bringing together young researchers to discuss, learn, and collaborate. Some senior scientists will be invited to share their ideas and encourage the discussion.

Contributions to any topic of scientific interest within computational science and engineering are welcome. The main areas, however, are the following:

- Computational Applied Mathematics,
- Computational Fluid Dynamics,
- Computational Materials Science,
- Computational Solids and Structural Mechanics,
- Scientific Computing.

As a conference designed by young researchers for young researchers, we will offer a variety of highlights such as a Science Slam, Journal Club, and numerous social events, thus nurturing the networking idea behind the conference. In addition, we will host the ECCOMAS Ph.D. Olympiad of 2015.

We are very happy to be able to announce that the event will be held in direct sequence with the AC.CES conference (www.ac-ces.rwth-aachen.de), organized by the graduate school AICES of RWTH Aachen. In contrast to the YIC and the GACM colloquium, the concept of the AC.CES is based on invited speakers with high international recognition in their particular fields. We will offer an optional combined package, giving participants the opportunity to profit from both conferences.

Please visit our website for further details: www.yic.rwth-aachen.de

CONFERENCE CHAIRPERSONS
STEFANIE ELGETI (CATS)
ELGETI@CATS.RWTH-AACHEN.DE
JAAN-WILLEM SIMON (IFAM)
JAAN.SIMON@RWTH-AACHEN.DE

Important Dates
Minisymposia submission deadline: October 24, 2014
Abstract submission deadline: January 16, 2015
Notification of abstract acceptance: March 6, 2015
Early registration deadline: May 15, 2015
The International Conference on Computational Plasticity (COMPLAS) was established in 1987, founded by the three chairmen Eugenio Oñate (Barcelona, Spain), Roger Owen and Ernie Hinton (both Swansea, UK); see Figures 1, 2. From then on it took place every two years, at the beginning occasionally every three years, but always at UPC in Barcelona, see Figure 3. Originally thought as a small specialty conference it grew up to over 400 delegates. From 2003 on it was integrated into the newly established series of ECCOMAS Thematic Conferences, being at the same time a special interest conference of the International Association for Computational Mechanics (IACM). The next one is scheduled for September 1-3, 2015.

Interesting to recognize the evolution of the topics during that period. Originally the conference was exclusively aligned to the area of the title, namely Computational Plasticity. Since the brand “COMPLAS” is a trademark in the meantime, it was reasonable, not changing the name. However the scope of the Conference has been substantially enlarged, adjusting to developments in academia and practice. It rather covers the subjects Material Modeling and Simulation in a very broad sense. Today syllables like multi, bio, nano can be recognized. New solution schemes appear in addition to the FEM, such as meshless and particle based methods.

Ernie Hinton, who was very much committed to the conference and its subjects, passed away in 1999. In the meantime Djordje Peric (Swansea, UK) and Benjamin Suarez (Barcelona; Spain), became co-chairman; the team is
headed by the local chairman (Figure 4). Due to the dedication of chairmen and a perfect management by Cristina Forace and her team, COMPLAS has a very personal flavor; quite a few people attended many of its meetings, see Figures 7 to 15.

Complas is a role model for an excellent conference with a high scientific standard taking place in a very friendly atmosphere.

*It is a true success story!*

Ekkehard Ramm
President of ECCOMAS
Ramm@IBB.Uni-Stuttgart.DE

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Name / Topic</th>
<th>Location</th>
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<tbody>
<tr>
<td>KomPlasTech</td>
<td>XXII Conference on Computer Methods in Materials Technology</td>
<td>Krynica-Zdrój, Poland</td>
<td>11-14 January</td>
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<tr>
<td>HONOM</td>
<td>European Workshop on High Order Nonlinear Numerical Methods for Evolutionary PDEs: Theory and Applications</td>
<td>Trento, Italy</td>
<td>16-20 March</td>
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<tr>
<td>SYMCOMP</td>
<td>International Conference on Numerical and Symbolic Computation: Developments and Applications</td>
<td>Faro, Portugal</td>
<td>26-27 March</td>
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<tr>
<td>Coupled Problems</td>
<td>VI International Conference on Coupled Problems in Science and Engineering</td>
<td>Venice, Italy</td>
<td>18-20 May</td>
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<tr>
<td>COMPDYN</td>
<td>5th International Conference on Computational Methods in Structural Dynamics and Earthquake Engineering</td>
<td>Crete, Greece</td>
<td>25-27 May</td>
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<tr>
<td>UNCECOMP</td>
<td>International Conference on Uncertainty Quantification in Computational Sciences and Engineering</td>
<td>Crete, Greece</td>
<td>25-27 May</td>
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<tr>
<td>CM3</td>
<td>Computational Multi Physics, Multi Scale and Multi Data in Transport Modeling, Simulation and Optimization</td>
<td>Jyväskylä, Finland</td>
<td>25-27 May</td>
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<tr>
<td>ICCCM</td>
<td>4th International Conference on Computational Contact Mechanics</td>
<td>Hannover, Germany</td>
<td>27-29 May</td>
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<tr>
<td>Rehab Structures</td>
<td>International Conference on Recent Advances in Rehabilitation and Sustainability of Structures</td>
<td>S. Miguel, Azores, Portugal</td>
<td>1-2 June</td>
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<tr>
<td>CFRAC</td>
<td>4th Conference on Computational Modeling of Fracture and Failure of Materials and Structures</td>
<td>Cachan, France</td>
<td>3-5 June</td>
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<tr>
<td>SMART</td>
<td>7th Conference on Smart Structures and Materials</td>
<td>S. Miguel, Azores, Portugal</td>
<td>3-6 June</td>
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<tr>
<td>ADMOS</td>
<td>VII International Conference on Adaptive Modeling and Simulation</td>
<td>Nantes, France</td>
<td>8-10 June</td>
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<tr>
<td>MARINE</td>
<td>VI International Conference on Computational Methods in Marine Engineering</td>
<td>Rome, Italy</td>
<td>16-17 June</td>
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<tr>
<td>Multibody Dynamics</td>
<td>2nd International Conference on Multibody Dynamics</td>
<td>Barcelona, Spain</td>
<td>29 June - 2 July</td>
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<tr>
<td>COMPLAS</td>
<td>XII International Conference on Computational Plasticity</td>
<td>Barcelona, Spain</td>
<td>1-3 September</td>
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<tr>
<td>COMPOSITES</td>
<td>V Conference on Mechanical Response of Composites</td>
<td>Bristol, UK</td>
<td>7-9 September</td>
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<tr>
<td>X-DMS</td>
<td>Extended Discretization Methods</td>
<td>Ferrara, Italy</td>
<td>9-11 September</td>
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<tr>
<td>EUROGEN</td>
<td>11th International Conference on Evolutionary and Deterministic Methods for Design, Optimization and Control with Applications to Industrial and Societal Problems</td>
<td>Glasgow, UK</td>
<td>14-16 September</td>
</tr>
<tr>
<td>PARTICLES</td>
<td>IV International Conference on Particle-based Methods</td>
<td>Barcelona, Spain</td>
<td>28-30 September</td>
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<tr>
<td>STRUCTURAL MEMBRANES</td>
<td>VII International Conference on Textile Composites and Inflatable Structures</td>
<td>Barcelona, Spain</td>
<td>19-21 October</td>
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<tr>
<td>VipIMAGE</td>
<td>V Conference on Computational Vision and Medical Image Processing</td>
<td>Santa Cruz de Tenerife, Spain</td>
<td>19-21 October</td>
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<tr>
<td>ICBT</td>
<td>International Conference on Biomedical Technology</td>
<td>Hannover, Germany</td>
<td>28-30 October</td>
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<td></td>
<td>3rd Workshop &quot;Reduced Basis, POD or PGD-based Model Reduction Techniques: a Breakthrough in Computational Engineering&quot;</td>
<td>Chamonix, France</td>
<td>4-6 November</td>
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**ECCOMAS**

**Thematic Conferences 2015 (2)**

**ECCOMAS**

**Special Interest Conferences 2015**

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<tr>
<td>AFRICOMP</td>
<td>4th African Conference on Computational Mechanics</td>
<td>Marrakech, Morocco</td>
<td>7-9 January</td>
</tr>
<tr>
<td>CMwM</td>
<td>2nd International Conference on Continuous Media with Microstructure</td>
<td>Lübeck, Poland</td>
<td>2-5 March</td>
</tr>
<tr>
<td>IGA</td>
<td>Isogeometric Analysis</td>
<td>Trondheim, Norway</td>
<td>1-3 June</td>
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Welcome to ECCOMAS Congress 2016 in Crete, Greece!

The European Community on Computational Methods in Applied Sciences (ECCOMAS) is pleased to announce the **ECCOMAS Congress 2016** to be held in Crete, Greece in June 5-10, 2016.

**Previous Editions of ECCOMAS Congresses:**

**Organizers**

[Logo: Greek Association for Computational Mechanics (GRACM)]

[Logo: Institute of Research and development for Computational Methods in Engineering Sciences (ICMES)]

**Minisymposia**

Members of the community are invited to organize Minisymposia in the different fields of the Congress. Participation of research teams from all parts of the world is welcomed and encouraged, as well as proposals of Minisymposia in emerging areas. Guidelines for the proposal and organization of Minisymposia and detailed information concerning the Congress may be found on the website: [http://www.eccomas2016.org](http://www.eccomas2016.org).

**Congress Venue**

The Congress will take place at the Creta Maris Convention Center, one of the largest convention centers in the Mediterranean (website: [http://www.conference-greece.com](http://www.conference-greece.com)). The complex is part of the Creta Maris Beach Resort overlooking Hersonisso Bay one of the most developed touristic resorts of Crete. The Convention Center is located 24 km away from Heraklion International Airport with many daily flights to and from Athens and regular and charter flights from 50 major cities of Europe and overseas.

![Image of the Congress Venue](image)

**Important Dates**

Deadline for submission of Minisymposia proposals: **January 31, 2015**
Deadline for presenting a one page abstract: **October 31, 2015**
Deadline for submitting the final contribution and early payment: **February 28, 2016**

For further information please visit [http://www.eccomas2016.org](http://www.eccomas2016.org) or contact the Congress Secretariat: [info@eccomas2016.org](mailto:info@eccomas2016.org).