

# expressions

**PGD-based "Computational Vademecum" for efficient design, optimization and control**

**F. Chinesta, A. Leygue & F. Bordeu, E. Cueto, D. Gonzalez, I. Alfaro, A. Ammar, A. Huerta & P. Diez** 

**Multiscale Modeling of Nano-Biosensors C.-S. Chen, Y.-C. Shih, C.-C. Chou, S.-W. Chang & C. Liou**

**Mortar Methods for Computational Contact Mechanics and General Interface Problems**

**A. Popp & W. A. Wall**

**The Particle Finite Element Method (PFEM) An Effective Numerical Technique for Multidisciplinary Problems in Engineering**

**E. Oñate, S.R. Idelsohn & Miguel A. Celigueta**

**Multigrid Techniques: 1984 Guide with Applications to Fluid Dynamics, Revised Edition Book Review by Dan Givoli**

**More CM Questions of the Month Dan Givoli**

**JSCES Japan USACM - USA AMCA - Argentina ABMEC- Brazil GACM - Germany KSCM - Korea Conference Diary**

*Bulletin for The International Association for Computational Mechanics*

> No 33 **July 2013**

н

Au

#### **Executive Council**

*President:* **G. Yagawa** Japan *Past Presidents:* **T. Hughes** U.S.A, **J.T. Oden** U.S.A., **E.Oñate** Spain**, A. Samuelsson**<sup><sup>†</sup> Sweden, **O.C. Zienkiewicz**<sup>†</sup> U.K.</sup> *Vice President (Americas):* **W.K. Liu** U.S.A*. Vice President (Asia-Australia):* **M. Yuan** China *Vice President (Europe-Africa):* **P. Wriggers** Germany *Secretary General:* **A. Huerta** Spain *Members:* **T. Belytschko** U.S.A, **J.S. Chen** U.S.A., **A. Coutinho** Brazil, **R. de Borst** Netherlands, **C. Farhat** U.S.A., **G. Hulbert** U.S.A., **S. Idelsohn** Argentina, **K. Kashiyama** Japan, **P. Ladevèze** France, **G.R. Liu** Singapore, **H. Mang** Austria, **M. Papadrakakis** Greece, **R. Ohayon** France, **B. Schrefler** Italy, **T. Tezduyar** U.S.A., **W. Wall** Germany

#### **IACM Honorary Members**

**E. Alarcon** Spain, **E. de Arantes e Oliveira** Portugal, **J. F. Besseling** Netherlands, **Y.K. Cheung** China, **C.K. Choi** Korea, **R. Dautray** France, **C.S. Desai** U.S.A., **S.J. Fenves** U.S.A., **R. Glowinski** U.S.A., **A. Jameson** U.S.A., **T. Kawai** Japan, **M. Kleiber** Poland, **P.K. Larsen** Norway, **C. Mota Soares** Portugal, **J. Périaux** France, **O. Pironneau** France, **K.S. Pister** U.S.A., **E. Stein** Germany, **G. Strang** U.S.A., **C.W. Towbridge** U. K., **E.L. Wilson** U.S.A., **W. Wunderlich** Germany, **G. Yagawa** Japan, **S. Valliappan** Australia, **Y. Yamada** Japan, **Y. Yamamoto** Japan, **W. Zhong** China

#### **IACM General Council**

**O. Allix** France **T. Aoki Japan E.R. Arantes e Oliveira** Portugal **G. Hulbert** U.S.A. **A.K. Ariffin** Malaysia **D. Aubry** France **F. Auricchio** Italy **E. Barbosa de las Casas** Brazil **J-L. Batoz** France **T. Belytschko** U.S.A. **N. Bicanic** U.K. **T. Bickel** U.S.A. **M. Bonnet** France **M. Borri** Italy **A.G. Boudouvis** Greece **T. Burczynski** Poland **M. Casteleiro** Spain **J. César de Sá** Portugal **A. Combescure** France **M. Cruchaga** Chile **J. S. Chen** U.S.A. **R. de Borst** Netherlands **L. Demkowicz** Poland **M. Doblaré** Spain **E. Dvorkin** Argentina **G. Etse** Argentina **C. Farhat** U.S.A. **C. Felippa** U.S.A. **I.N. Figueiredo** Portugal **J. Fish** U.S.A. **K. Fujii** Japan **Z. Gaspar** Hungary **S. Ghosh** U.S.A. **J.M. Goicolea** Spain **M. Goldschmidt** Argentina **R. Haber** U.S.A. **I. Hagiwara** Japan **I. Harari** Israel **R. Himeno** Japan

**A. Huerta** Spain **T. Hughes** U.S.A. **S. Idelsohn** Argentina **W. Ju** U.S.A. **W. Kanok-Nukulchai** Thailand **K. Kashiyama** Japan **M. Kawahara** Japan **S. Kawata** Japan **M. Kleiber** Poland **S. Koshizuka** Japan **T. Kvamsdal** Norway **H.G. Kwak** Korea **P. Ladevèze** France **R. Larsson** Sweden **T. Laursen** U.S.A. **G. R. Liu** Singapore **W. K. Liu** U.S.A. **T. Lodygowski** Poland **P.R.M. Lyra** Brazil **Y. Matsumoto** Japan **G. Meschke** Germany **N. Miyazaki** Japan **N. Moës** France **C. Mota Soares** Portugal **K. Nakahashi** Japan **K. Nakajima** Japan **N. Nishimura** Japan **S. Obayash**i Japan **J. T. Oden** U.S.A. **R. Ohayon** France **H. Okuda** Japan **X. Oliver** Spain **E. Oñate** Spain **K. Ootomi** Japan **J. Orkisz** Poland **M Oshima** Japan

**J. Pamin** Poland **M. Papadrakakis** Greece **U. Perego** Italy **J.C.F. Pereira** Portugal **P. Pinsky** U.S.A. **E. Ramm** Germany **E. Rank** Germany **J. N. Reddy** U.S.A. **S. Reese** Germany **E. Sacco** Italy **J. Soric** Croatia **P. Steinmann** Germany **K. Suzuki** Japan **N. Takano** Japan **N. Takeuchi** Japan **T. Taniguchi** Japan **C. Taylor** U.S.A. **J.A. Teixeira de Freitas** Portugal **K. Terada** Japan **T. Tezduyar** U.S.A. **S. Valliappan** Australia **W. Wall** Germany **T. Watanabe** Japan **K. Willam** U.S.A. **B. Wohlmuth** Germany **P. Wriggers** Germany **T. Yabe** Japan **G. Yagawa** Japan **T. Yamada** Japan **M. Yamamoto** Japan **Y.B. Yang** Taiwan **S. Yoshimura** Japan **M. Yuan** China **K. Yuge** Japan **H. Zhang** China **Y. Zheng** China **T. Zohdi** U.S.A.

*Members of the Executive Council, Honorary Members & Presidents of Affiliated Associations are also members of the General Council*

**D.R.J. Owen** U.K.

#### **IACM Membership - Fee**

The annual fee for direct individual membership of IACM is 25 US dollars. For affiliated organisations the membership fee is reduced to 10US dollars. The Bulletin and a discount on IACM supported activities (congress, seminars, etc.) are some of the benefits of the membership.

#### **IACM Expressions**

**Published by:** The International Association for Computational Mechanics (IACM)<br>**Editorial Address:** IACM Secretariat, Edificio C1, Campus Norte UPC, Gran Capitán sa IACM Secretariat, Edificio C1, Campus Norte UPC, Gran Capitán s/n, 08034 Barcelona, Spain. *Tel:* (34) 93 - 405 4697 *Fax*: (34) 93 - 205 8347 *Email*: iacm@cimne.upc.edu *Web*: www.iacm.info

Editor: Eugenio Oñate **Production Manager**: Diane Duffett *Email:* diane.duffett@telefonica.net **Advertising**: For details please contact Diane Duffett at the IACM Secretariat.

## *Listed in order of affiliation*

**U.S.A.** (USACM) *T. Zohdi United States Association for Computational Mechanics*  **Argentina** (AMCA) *Asociación Argentina de Mecánica Computacional*  **PR China** (CACM) *M.W. Yuan Chinese Association of Computational Mechanics*  **Italy** (AIMETA) *M. Cuomo Associazione Italiana di Meccanica Teorica e Applicata* **Denmark, Estonia, Finland, Iceland, Latvia, Lithuania, Norway, Sweden** (NoACM) *T. Kvamsdal The Nordic Association for Computational Mechanics* **Japan** (JSCES) *K. Kashiyama Japan Society for Computational Engineering and Science*  **Japan** (JACM) *S. Yoshimura Japan Association for Computational Mechanics* **Spain** (SEMNI) *X. Oliver Sociedad Española de Métodos Numéricos en Ingeniería* **Germany** (GACM) *Wolfgang A. Wall German Association of Computational Mechanics*  **France** (CSMA) *F. Chinesta Computational Structural Mechanics Association* **U.K.** (ACME) *C. Sansour Association for Computer Methods in Engineering*  **Greece** (GRACM) *G.E. Stavroulakis The Greek Association of Computational Mechanics*  **Austria, Croatia, Hungary, Poland, Slovenia, The Czech Republic** (CEACM) *P. Polach Central-European Association for Comp. Mechanics*  **Poland** (PACM) *J. Pamin Polish Association for Computational Mechanics* **Chile** (SCMC) *F Perazzo Sociedad Chilena de Mecánica Computacional*  **Israel** (IACMM) *D. Givoli Israel Association of Computational Methods in Mechanics* **Portuga**l (APMTAC) *C. Mota Soares Portuguese Society of Theoretical, Applied & Computational Mechanics* **Australia** (AACM) *S. Valliappan Australian Association of Computational Mechanics* **Brazil** (ABMEC) *G. Farias Moita Brazillian Association for Comp. Methods in Engineering*  **Mexico** (AMMNI) *G. Valdés Asociación Mexicana de Métodos Numéricos en Ingeniería* **Korea** (KACM) *H-G. Kwak Korean Association on Computational Mechanics* **Korea** (KSCM) *S.K. Youn Korean Society of Computational Mechanics* **Thailand** (TSCM) *Thailand Society for Computational Mechanics* **Singapore** (SACM) *Z.S. Liu Singapore Association for Computational Mechanics*  **Netherlands** (NMC) *D.H. van Campen Netherlands Mechanics Committee* **Malaysia** (MACM) *A.K. Ariffin Malaysian Association for Computational Mechanics*  **Serbia** (SSCM) *M. Kojic Serbian Association for Computational Mechanics*  **Taiwan** (ACMT) *Y.B. Yang Taiwan Association for Computational Mechanics Taiwan*  **Hong Kong** (KHACM) *A.Y.T. Leung Hong Kong Association of Computational Mechanics* **Colombia** (ACMENICA) *D.L. Linero Segrera Colombian Association for Numerical Methods in Engineering and Applied Sciences* **Venezuela** (SVMNI) *M. Cerrolaza Venezuelan Society for Numerical Methods in Engineering*

**IACM members are invited to send their contributions to the editors.**

**Views expressed in the contributed articles are not necessarily those of the IACM.**



Computational mechanics is one of the faster growing technologies and gas extraction. The challenging problems posed by these industries are of considerable complexity and include the study of oil and gas flow in porous and fractured geological media, new drilling techniques, stability of drill strings, drill-bit interaction, wear of cutting tools, transport of cuttings and gas bubbles in boreholes and efficient and safe control of the drilling and extraction operations, to list just a few.

The solution of above problems requires advanced mathematical models and computational methods for multi-scale analysis of multiphase flow in porous media, fluid-soil-structure interaction, fracture of soil and rock, particulate non Newtonian flows and optimal control, among others. Many of these computational techniques are indeed not new. However their application in the context of oil and gas extraction poses new challenges that will require innovative and ad-hoc computational mechanics procedures.

The interest in the oil and gas field has increased in recent years due to the fast expansion of the hydraulic fracturing technology (commonly known as "fracking" ). Fracking is a technique in which usually a large amount of water is mixed with sand and/or chemicals. This mixture is injected at high pressure into faults to release petroleum, natural gas, or other substances for extraction. This type of fracturing creates fractures from a wellbore drilled into reservoir rock formations.

The first experimental use of hydraulic fracturing was in 1947, and the first commercially successful applications were in 1949. As of 2010, it was estimated that 60% of all new oil and gas wells worldwide were being hydraulically fractured. As of 2012, 2.5 million hydraulic fracturing jobs have been performed on oil and gas wells worldwide, more than one million of them in the United States.

Proponents of hydraulic fracturing point to the economic benefits from the vast amounts of formerly inaccessible hydrocarbons the process can extract. Opponents point to potential environmental impacts, including contamination of ground water, and the health effects of these. For these reasons hydraulic fracturing has come under international scrutiny, with some countries suspending or banning it.

Another topic of much debate is the effect of oil and gas extractions in provoking subsidence and co-lateral seismic effects due to the collapse of internal cavities in the ground induced by the extraction process.

The above topics are obviously of upmost importance, as they can drastically change the way energy resources of today are dealt with and improved in the future. This is indeed a field where computational mechanics has a lot to say to help design safer, environmentally friendly and efficient and oil and gas extraction procedures.

Let me finally remind you that the next World Congress on Computational Mechanics (WCCM) will be held on July 20-25, 2014 in Barcelona, Spain. This congress will be held in conjunction with the ECCOMAS conferences on solids and structures and fluid dynamics. So far some 260 specialized Simposia have been proposed covering many different field in engineering and applied sciences. Numbers so far indicate that WCCM2014 can be a record in participation. We look forward to seeing you at this important event.

> *Eugenio Oñate* Editor of IACM Expressions

## PGD-based "Computational Vademecum" for efficient design, optimization and control

*F. Chinesta GeM, UMR CNRS - Centrale Nantes & Institut Universtaire de France and A. Leygue & F. Bordeu GeM @ Centrale Nantes E. Cueto, D. Gonzalez & I. Alfaro 3A @ University of Zaragoza A. Ammar Arts et Métiers ParisTech A. Huerta & P. Diez LaCaN @ UPC Barcelona*

*by*

**Despite the impressive progresses**<br>attained by simulation capabilities and techniques, some challenging problems remain today intractable. These problems, that are common to many branches of science and engineering, are of different nature. Among them, we can cite those related to high-dimensional models, on which mesh-based approaches fail due to the exponential increase of degrees of freedom. Other challenging scenarios concern problems requiring many direct solutions (optimization, inverse identification, uncertainty quantification …) or those needing very fast solutions (real time simulation, simulation based control …).

We are developing a novel technique, called Proper Generalized Decomposition (PGD) based on the assumption of a separated form of the unknown fields that has demonstrated its capabilities in dealing with high-dimensional problems overcoming the strong limitations of classical approaches. But the main opportunity given by this technique is that it allows for a completely new approach for addressing standard problems, not necessarily high dimensional. Many challenging problems can be efficiently cast into a multidimensional framework opening new possibilities to solve old and new problems with strategies not envisioned until now. For instance, parameters in a model can be set as additional extra-coordinates of the model. In a PGD framework, the resulting model is solved once for life, in order to obtain a general solution that includes all the solutions for every possible value of the parameters, that is, a sort of "Computational Vademecum". Under this rationale, optimization of complex problems, uncertainty quantification, simulation-based control and real-time simulation are now at hand, even in highly complex scenarios, by combining an off-line stage in which the general PGD solution, the "vademecum", is computed, and an on-line phase in which, even on deployed, handheld, platforms such as smartphones or tablets, real-time response is obtained as a result of our queries. See [1] for a recent review on this topic.

#### **Motivation**

It is now well known that the human brain consumes 4 watts for performing some tasks for which today's computers would require the power of several nuclear plants. It is then clear that our computers and algorithms for addressing the models encountered in science and engineering are definitively suboptimal.

Up to now, the solution of complex models, preferably fast and accurate, is addressed by using high performance computing on hyper powerful computing platforms. Obviously most exciting applications will require as much computational power as possible, and consequently further advances in hardware and software for high-performance computing will be necessary. But at the same time, there is a need for a new generation of simulation techniques, beyond high-performance computing and nowadays approaches (most of them proposed 40 years ago), to improve efficiency or to solve problems never until now solved.

Today many problems in science and engineering remain intractable, in spite of the impressive progresses attained in modeling, numerical analysis, discretization techniques and computer science during the last decade, because their numerical complexity, or the restrictions imposed by different requirements (realtime on deployed platforms, for instance) make them unaffordable for today's technologies.

We can enumerate different challenging scenarios for efficient numerical simulations:

- The first one concerns models that are defined in high dimensional spaces: quantum chemistry, kinetic theory descriptions, the chemical master equation, …;
- Simulation-based control, where classical coarse transfer functions should be substituted by richer PDE-based models;
- Parametric modeling, inverse identification, and process or shape optimization, usually require, when approached with standard techniques,

the direct computation of a very large number of solutions of the concerned model;

- Dynamic Data-Driven Application Systems (DDDAS) constitute nowadays one of the most challenging applications of simulation-based Engineering Sciences. DDDAS entails the ability to dynamically incorporate additional data into an executing application, and in reverse, the ability of an application to dynamically steer the measurement process;
- Real time simulations are needed in many applications. One of the most challenging situations is that of haptic devices, where forces must be translated to the peripheral device at a rate of 500 Hz;
- Augmented reality is another area in which efficient (fast and accurate) simulation is urgently needed. The idea is supplying in real time appropriate information to the reality perceived by the user;
- The consideration of variability, randomness and uncertainty is a priority for the next decade.

While the previous list is by no means exhaustive, it includes a set of problems with no apparent relationship between them that can however be treated in a unified manner as will be shown in what follows. Their common ingredient is our lack of capabilities (or knowledge) to solve them numerically in a direct, traditional way.

#### **Fast calculations from a historical perspective**

Throughout history, men have developed many devices for giving fast responses to a variety of questions. Thus, abaci were used 2700 years B.C. in Mesopotamia. The abacus was a sort of counting frame primarily used for performing arithmetic calculations. It was in use centuries before the adoption of the written modern numeral system and is still widely used.

However, the initial arithmetic needs were rapidly complemented with more complex necessities. We are considering some few variants:

- Charts appeared for graphical representation of data with multiple meanings. In general a chart is graphical, containing very little text, since humans infer meaning from pictures quicker than from text. A particular variant of charts is the Nomogram.
- Nomography, is the graphical representation of mathematical relationships or

laws. It was used extensively for many years to provide engineers with fast graphical calculations of complicated formulas to a practical precision. Thus, a nomogram can be considered as a graphical calculating device.

The former tools allowed for fast calculations and data manipulations. Nomograms can be easily constructed when the mathematical relationships that they express are explicit, eventually non-linear. In those cases it is easy to represent some outputs as a function of some inputs. The calculation of these data representations was performed off-line and then used on-line in many branches of engineering sciences for design and optimization.

However, the former procedures fail when addressing more complex scenarios. Sometimes engineers manipulate systems of complex coupled non-linear partial differential equations, whose solution for each possible combination of the values of the parameters that they involve is simply unaffordable from nowadays computational availabilities. In these cases experiments or expensive computational solutions are performed for some values of the model parameters, from which a simplified model linking the inputs to the outputs of interest is elaborated. These simplified models have different names: surrogate models, metamodels, response surface methodologies, ... Other associated tricky questions are the one that concerns the best sampling strategy and also the one concerning the appropriate interpolation techniques for estimating the response at any point.

*Figure 1: Particularizing online on a tablet the general parametric thermal solution*



Recently model order reduction opened new possibilities. First, proper orthogonal decompositions (POD) allows extracting the most significant characteristics of the solution, that can be then applied for solving models slightly different to the one that served to define the reduced approximation basis. There is an extensive literature. The extraction of the reduced basis, its adaptation when addressing scenarios far from the ones considered when constructing the reduced basis, and the error estimation and control, are some points of intensive research.

*Figure 2: Towards real time surgical simulations based on parametric PGD-based vademecums*



Another family of model reduction techniques lies in the use of reduced basis constructed by combining a greedy sampling algorithm and an a priori error indicator. It needs for some amount of off-line work but then the reduced basis can be used on-line for solving different models with a control of the solution accuracy because the availability of error bounds. When the error is inadmissible, the reduced basis can be enriched by considering again the same greedy algorithm.

*Figure 3:* Add-on developed for the open source post-processing code ParaView. The three sliders on the bottom-right menu control, respectively, the Poisson coefficient, Young's modulus and thickness

An alternative approach has its foundations in the separated or tensor product representations. Separated representations were introduced in the field of computational mechanics in the 80s by Pierre Ladeveze [2] that proposed a



space-time separated representation of transient solutions in strongly non-linear models, defining a non-incremental integration procedure. Later, separated representations were employed in the context of stochastic modeling for separating the stochastic and the deterministic parts [3] as well as for solving multidimensional models suffering the so-called curse of dimensionality, some of them never solved before [4]. The techniques making use of separated representations computed on the fly were called Proper Generalized Decompositions -- PGD --.

We proposed some years ago using the PGD as an efficient multidimensional solver that allows introducing model parameters (boundary conditions, initial conditions, geometrical parameters, material and process parameters ...) as extra-coordinates. Then by solving only once and off-line the resulting multidimensional model we have access to the parametric solution that can be viewed as a sort of handbook, virtual chart or vademecum than can be then used on-line. These vademecums can be viewed as a sort of modern monograms related to complex multiparametric partial differential equations.

#### **Using computational vademecums**

*Figure 1* illustrates the use of an ATP (automated tape placement) vademecum in composite manufacturing processes. In this process a moving laser with of power P and line velocity V is melting the incoming tape on the substrate surface. The heat conduction inside the part depends on at least three contact resistances because the different degree of consolidation of the different layers. The temperature field in such processes is significantly affected by many material and process parameters. In this context the process optimization depends on the optimal choice of at least 5 parameters, the laser power, the line velocity and the three contact resistances. The identification of the thermal resistances and the evaluation of the process window is a delicate task, traditionally time consuming.

We solved the thermal model by introducing the laser power, the line velocity and the three thermal resistances as extracoordinates. Then, the computed parametric solution (obtained by solving the associated 7D non-linear partial differential equation) allowed an easy and fast inverse identification of the thermal resistances. Finally, different scenarios could

be evaluated and compared in real time, allowing the definition of the process window and even the process optimization and control in real time on a tablet. A picture of such a computational device that has been successfully transferred to the industry is depicted in *Figure 1* where process conditions can be modified in real time by using the horizontal sliders located on the lower part of the window. The degrees of consolidation and thermal degradation are given instantaneously in the upper part of the application window.

Another application concerns surgical simulators that must provide feedback response frequencies higher than 500 Hz. This means that we must solve problems involving material and geometrical nonlinearities close to one thousand times per second. It is now clear that the use of model reduction seems to be an appealing alternative for reaching such performances. In this context we proposed considering the applied load and its point of application as extra-coordinates, allowing the off-line calculation of the parametric solution, that is, the calculation of the displacement and stress fields for any load applied at any position. This parametric solution computed off-line that can be viewed as a sort of computational vademecum, is then exploited in real time (see *Figure 2*) even on mobile devices (smartphones, tablets …). As soon as the load is modified (in magnitude or position) we do not need to solve again the resulting mechanical model but only particularize the available parametric solution. This off-line / on-line strategy allows real time

feedbacks opening new routes for real time simulations.

*Figure 3* illustrates the use of a computational vademecum for the design of a mechanical system in which geometrical parameters defining the part shape and geometry, the material parameters (Young's modulus and Poisson's coefficient) were considered as extracoordinates. Then, the computational vademecum can be used online for exploring the whole design space and linked to a library of material properties.

Finally, *Figure 4* illustrates the possible use of these computational vademecums in the context of enriched learning. The vademecum can be integrated in electronic books that become a sort of virtual labs in which students can explore dynamically and in real time different scenarios.

The interested reader can refer to [1][5] and the references therein for additional details on the computation of multiparametric solutions when considering (i) material parameters; (ii) boundary conditions; (iii) initial conditions; and (iv) geometrical parameters as extra-coordinates.

This route makes possible a variety of applications in the domain of real time design, optimization, inverse identification and simulation based control of materials, processes and structures.  $\bullet$ 

#### *Figure 4:*

*Implementation of the technique described before on an iPhone. Simple formats such as the epub open format, that enables javascript, suffices for implementing this technique in enriched learning applications*



#### **Acknowledgments**

Authors acknowledge the different PhD students involved in the development of the Proper Generalized Decomposition and the associated "Computational Vademecums", in particular Ch. Ghnatios, B. Bognet, J.V. Aguado, F. Poulhaon, S. Niroomandi, D. Modesto, S. Aghighi. They also acknowledge the support of Spanish and French ministries through grants CICYT-DPI2011-27778-C02-01/02 and ANR COSINUS 2010 SIMDREAM, the « Institut Universitaire de France » - IUF. Finally they also acknowledge the support of many industries through different research projects and industrial chairs, in particular EADS, AIRBUS, ASTRIUM, AEROLIA, ESI …

#### **References**

- [1] *F. Chinesta, A. Leygue, F. Bordeu, J.V. Aguado, E. Cueto, D. Gonzalez, I. Alfaro, A. Ammar, A. Huerta*. **Parametric PGD based computational vademecum for efficient design, optimization and control.** Archives of Computational Methods in Engineering, 20/1, 31-59, 2013.
- [2] *Ladevèze*. **The large time increment method for the analyze of structures with nonlinear constitutive relation described by internal variables**. Comptes Rendus Académie des Sciences Paris, 309, 1095-1099, 1989.
- [3] *A. Nouy*. **Recent developments in spectral stochastic methods for the solution of stochastic partial differential equations**. Archives of Computational Methods in Engineering, 16/3, 251-285, 2009.
- [4] *A. Ammar, B. Mokdad, F. Chinesta, R. Keunings.* **A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modeling of complex fluids.** Journal of Non-Newtonian Fluid Mechanics, 139, 153-176, 2006.
- [5] *F. Chinesta, P. Ladeveze, E. Cueto*. **A short review in model order reduction based on Proper Generalized Decomposition.** Archives of Computational Methods in Engineering, 18, 395-404, 2011.

## Multiscale Modeling of N ano-Biosensors

*by Chuin-Shan (David) Chen, Yu-Ching Shih, Chia-Ching Chou, Shu-Wei Chang, Crystal Liou National Taiwan University*

Ultrasensitive nano-biosensor related<br>research is a vital and rapidly developing field owing to its potential social and economic impact. For example, the technology shows promise in detecting disease in an early stage; monitoring contaminants and bioweapons in air, water and soil; reducing food borne infection; and benefiting healthcare, biomedical technology, and clinical analysis. Chemo-bio-mechanical phenomena in biosensing offer an enticing opportunity for researchers in the field of computational mechanics to investigate these phenomena with methodologies that have not previously been exploited, and to provide new insights into the design of nextgeneration ultrasensitive nano-biosensors.



The microcantilever is one of the most promising ultrasensitive nano-biosensors [1]. It is highly portable and supports labelfree molecular recognition measurement with an ultra-high sensitivity. With the advance of the micro/nano electromechanical systems (MEMS/NEMS) technology, variously shaped microcantilevers can be now routinely fabricated in batches *(Figure 1)*. The device has been used to detect biomolecules (such as DNA and proteins associated with cancer or other diseases), chemicals (such as explosives and glucose), and ionic species (such as calcium ions). It is thus rather surprising to note that the theoretical description and predictive modeling of these devices are not well developed, and lag behind advances in fabrication and applications [2-4].

At its simplest, the key components of biosensors consist of a sensing layer, a transducer and a recorder *(Figure 2)*. The sensing layer is normally a receptor which can bind or interact with a target analyte molecule. The transducer transforms the signals and the recorder is a read-out system. For example, microcantilever biosensors can translate bio-recognition events into mechanical





#### *Figure 1:*

*Scanning electron micrograph of various shapes of a gold-coated microcantilever fabricated using MEMS/NEMS technology*



*Figure 2: The three key components of biosensors: a sensing layer for molecular recognition, a transducer for signal translation, and a recorder for processing*

motion ranging from a few to hundreds of nanometers. The theoretical modeling challenge thus lies in how to couple molecular interactions with a continuum description: a daunting but rewarding intellectual challenge with great potential. In this article, we will highlight some recent progress made in predicting the macroscopic response of microcantilevers through the microscopic fidelity of molecular interactions.

#### **Top-down Information Passage**

One simple way to couple a continuum description with first principles density functional theory (DFT) calculations or classical molecular dynamics/statics (MD) simulations is to link atomic contributions with kinematic constraints imposed by continuum mechanics [2, 3]. For example, if we consider a differential element in a microcantilever subjected to a uniform curvature, we can take the derivative of the total potential energy with respect to curvature and directly relate the Stoney formula for surface stress to atomic positions and atomic forces originating from the local rearrangement of surface atoms as well as charge redistribution induced by ligand adsorption.

*Figure 3* shows a calculated charge distribution of an alkanethiol  $(SC_4H_9)$  adsorbed on a gold film. Detailed DFT calculations allow us to capture the binding process between the sulfur and gold atoms. Binding of the sulfur atom alters the atomic positions as well as charge distribution of the gold atoms in a few surface layers. Consequently, it induces surface stresses and



*Figure 3: Charge distribution from DFT calculations of an alkanethiol (SC4H9) adsorbed on a gold film*



#### *Figure 4:*

*(a)*

*Adsorption of cSALF onto a microcantilever surface. (a) cSALF (pink ribbon) above linkers (ochre) and gold surface (yellow) surrounded by solution (cyan) and (b) snapshots of the adsorption process (the solution is not shown for clarity).* 





bends the microcantilever.

#### *Figure 5:*

*Charge difference slicing through the surface gold atoms upon methanethiolate (SCH3) adsorption. In (b) methanethiolate is not shown for clarity* Similarly, we can use MD simulations to capture bio-molecular recognition with length and time scales beyond the reach of DFT calculations. For example, consider a cyclic shrimp anti-lipopolysaccharide factor (cSALF), an antimicrobial peptide that can affect the infection of grouper nervous necrosis virus [5]. *Figure 4* shows snapshots of cSALF adsorbed onto thiol group linkers from molecular dynamics simulations. Again the induced surface stress can be predicted from the scheme imposed with a uniform curvature constraint [2].

#### **Bottom-up Information Passage**

The simple kinematically constrained method provides a pathway to study rich physics for adsoption-induced surface stress. However, we sometimes do not know or do not want to assume the deformation field a priori. For example, to maximize the portability of the microcantilever biosensors, an embedding piece of piezoresistive material or a metal-oxide semiconductor field effect transistor (MOSFET) is often used to detect the



deflection-induced strain due to biomolecular binding. As they are directly embedded in the microcantilever, there is no need for an extra



instrument for deflection detection. Strain distributions in a microcantilever are not homogeneous and cannot be resolved by simply imposing a uniform curvature deformation. We thus need to perform detailed DFT or MD calculations in a representative volume at the microscopic level and use this information to solve the desirable macroscopic response with finite element (FE) analysis.

Let us take DFT and FE coupling to illustrate this bottom-up information passage scheme. By using DFT calculations, we can obtain the spatial distribution of electrons in a representative volume before and after molecular adsorption. *Figure 5* shows a charge difference slicing through the surface gold atoms upon methanethiolate  $(SCH<sub>3</sub>)$  adsorption. Charge removal occurs in the blue region where the sulfur atom binds to the surface, indicating an induced compressive surface stress. Using the Hellmann-Feynman theorem, all the forces and stresses in the representative volume can be obtained from the DFT calculations. These prescribed forces and stresses can then be applied to a finite element model of a microcantilever. *Figure 6* shows the deformation and the strain distribution of a 3D microcantilever with these prescribed stresses and forces. It is not surprising to observe that the maximum strain occurs at the clampedend of the microcantilever, indicating a good location to embed a piezoresistor or MOSFET. Using the bottom-up information passage scheme, we open a new gateway for simulation-based modeling and design to optimize the signal to noise (S/N) ratio of nano-biosensors.

#### **References**

- [1] *J.R. Heath, M.E. Davis, L. Hood*, **Nanomedicine Targets Cancer**, Scientific American, February (2009), 300, 44-51.
- [2] *C.-S. Chen, C.-C. Chou, S-W. Chang*, **Multiscale Analysis of Adsorption-induced Surface Stress of Alkanethiol on Microcantilever**, Journal of Physics D: Applied Physics, 46 (2013), 035301.
- [3] *C.-S. Chen, S. Kuan, T.-H. Chang, C.-C. Chou, S.-W. Chang, L.-S. Huang*, **Microcantilever Biosensor: Sensing Platform, Surface Characterization, and Multiscale Modeling**, Smart Structures and Systems, 8 (2011) 1, 17-37.
- [4] *Y.-C. Shih, C.-S. Chen, K.-C. Wu*, **Chain Length Effect on Surface Stress of Alkanethiolates Adsorbed onto R30° Au(111) Surface: a van der Waals Density Functional Study**, Journal of Mechanics (2013), accepted.
- [5] *S. Kuan, S.-C. Chi, Y.-J. Cheng, T.-J. Chia, L.-S. Huang*, **Binding Kinetics of Grouper Nervous Necrosis Viruses with Functionalized Antimicrobial Peptides by Nanomechanical Detection**, Biosensors and Bioelectronics, 31 (2012) 1, 116–123.

#### **Conclusion**

We have shown two simple schemes inspired by information passage from one scale to another to predict the surface stress and strain distribution of microcantilevers through the microscopic fidelity of molecular interactions. We finally remark that these scales should be seamlessly coupled and our preliminary work using a 3D quasicontinuum method (Figure 7) has shown a promising future for concurrent coupling of nano-biosensor modeling.  $\bullet$ 

*Figure 7: Simple 3D quasicontinuum model for concurrent coupling of nano-biosensor modeling*



#### **9** iacm expressions 33/13

*Figure 6: Deformation and strain distribution of a microcantilever with prescribed stresses and forces, obtained from DFT calculations*

# Mortar Methods for Computational Contact Mechanics and General Interface Problems

*by Alexander Popp and Wolfgang A. Wall Technische Universität München [popp,wall]@ lnm.mw.tum.de*

Mortar finite element methods are of great relevance as a non-conforming discretization technique in various singlefield and multi-field applications and have seen a significant thrust of research over the last decade. In computational contact mechanics, the mortar approach allows for a variationally consistent treatment of nonpenetration and frictional sliding constraints despite the inevitably non-matching interface meshes. Other problem classes, such as flow problems or fluid-structure interaction (FSI), also benefit from the increased modeling flexibility provided by mortar methods. This contribution gives a review of the most important features of non-conforming finite element discretization based on mortar methods with a special emphasis on the choice of discrete Lagrange multiplier spaces, efficient solution algorithms in contact mechanics and high performance parallel computing.

#### *The origins of mortar methods*

Originally introduced as a domain decomposition technique for spectral elements in [1], mortar methods are nowadays also widely used as a discretization scheme within finite element formulations for many different problem classes. First investigations on mortar finite element methods were typically performed for model problems of Laplace type, e.g. the Poisson equation, and formulated as a non-conforming variational problem with the coupling constraints directly introduced into the global solution space. Yet, an alternative formulation soon became more popular, which is not based on a constrained solution space, but rather introduces Lagrange multipliers in the sense of constrained minimization, thus leading to a typical saddle point formulation [2]. Details of both approaches and their rigorous mathematical formulation can be found in [3].

#### *What mortar methods are all about*

The mortar approach is characterized by an imposition of interface constraints in a weak sense and by the possibility to prove its mathematical optimality. This means that suitable inf-sup conditions and a priori error estimates for the consistency error and the best approximation error have been established for the most widely used finite element discretizations and for different choices of the discrete Lagrange multiplier space. An intuitive application of mortar methods in solid mechanics are so-called tied contact problems *(Figures 1 & 2)*. If considering first-order finite elements and uniform mesh refinement as an example, the optimal spatial convergence of order  $O(h^2)$  measured in the  $L^2$ -norm is preserved by mortar methods, despite the fact that non-conforming interfaces are involved. Establishing optimal a priori error bounds for unilateral contact problems is more intricate due to the reduced regularity of the solution. However, the optimality of mortar methods can also be proven in that context.

#### *Choice of the discrete Lagrange multiplier space*

Especially the choice of the discrete Lagrange multiplier space is an essential question with great implications on the algorithmic realization of mortar methods. So-called *standard* mortar methods, where the discrete Lagrange multipliers are simply chosen from the trace space of the underlying primary variables, suffer from a serious drawback: they generate high computational costs due to the global character of the resulting interface coupling conditions, see [3] for a detailed explanation. When considering again a tied contact problem of solid mechanics as example, the interface coupling

*Figure 1: A tied contact (mesh tying) example from solid dynamics: The two non-conforming sub-structures are connected with a mortar finite element approach*





displacement magnitude

condition after mortar finite element discretization reads

$$
Dd_1 = Md_2 \tag{1}
$$

where  $d_1$  and  $d_2$  contain the discrete displacement degrees of freedom on both sides of the interface. **D** and **M** are the so-called discrete mortar matrices, which basically contain entries of mass matrix type. Thus, a linear system of equations of interface size needs to be solved whenever evaluating the mortar coupling conditions. However, this issue can be completely resolved by introducing so-called *dual* Lagrange multiplier spaces as initially proposed in [4], which are constructed based on a biorthogonality condition such that the interface coupling conditions reduce to purely local constraints *(Figure 3)*. Algebraically, this advantageous property can be observed by the mortar matrix **D** in (1) reducing to a diagonal matrix. This allows for very efficient condensation procedures of the discrete Lagrange multiplier degrees of freedom, which completely remove the undesirable saddle point structure of the underlying systems.

#### *Computational contact mechanics*

The approach outlined above has been applied very successfully to impose unilateral interface constraints for small deformation contact analysis and later also for finite deformation contact analysis, see e.g. [5-7]. Especially when considering finite deformations and large frictional sliding motions, the complexity of the underlying physics and numerics increases significantly, since now relative motions occur at the coupling interface *(Figure 4)*. This not only requires a continuous re-evaluation of the discrete mortar matrices introduced in (1) in the current configuration, but in the context of implicit time stepping schemes and Newtonbased nonlinear solution methods also a consistent linearization of all deformationdependent quantities, such as surface normals and tangents as well as projection and mesh intersection procedures. Yet, when carefully considering these additional complexities, mortar methods exhibit a far superior robustness as compared with traditional contact discretizations.

#### *Semi-smooth Newton methods*

To eventually solve the fully discretized system of nonlinear algebraic equations and inequality constraints in each time step, we aim at using standard Newton– Raphson iterations despite the underlying non-smoothness of the discrete contact and friction laws. This can be achieved by re-interpreting the well-known concept of



*equality* conditions which equivalently replace the full sets of contact *inequality* conditions (e.g. Karush-Kuhn-Tucker conditions as for non-penetration or Coulomb friction). For the sake of brevity, we do not discuss the resulting global solution algorithm here, but the interested reader is referred to the numerous recent contributions on this topic, see e.g. [5-7]. The major advantage of the proposed solution algorithm is that all sources of nonlinearities, including finite deformations, nonlinear material behavior as well as frictional contact itself (i.e. the search for the active contact set and for stick and slip regions), can be treated within one single iterative scheme. Numerical investigations have shown that the semi-smooth Newton approach allows for a very efficient treatment of finite deformation contact problems, also including frictional sliding. Even for relatively large step sizes and fine contacting meshes, the correct active set is usually

*Figure 4:*

*Torus impact in 3D as an example for the successful application of mortar methods for unilateral contact problems including finite deformations and frictional sliding*

 **11** iacm expressions 33/13



#### *Figure 5:*

*Typical convergence behavior of the semi-smooth Newton method in terms of the nonlinear residual (left) and in terms of the active contact set (right). The shaded regions indicate that the active contact set is already fully converged in these steps*

> found after only a few Newton steps. Once the sets remain constant, quadratic convergence of the Newton-Raphson scheme is obtained in the limit owing to the underlying consistent linearization *(Figure 5).*

#### *General interfaces and multiphysics problems*

Thermomechanical coupling models accounting for frictional heat disspation and simple wear models can readily be included into the described contact algorithms. Recently, the focus of research in the field of mortar methods and dual Lagrange multiplier interpolation has been extended towards other single-field applications beyond solid mechanics and especially to coupled multiphyics problems. A computational framework for mortar-based fluid-structure interaction has been proposed in [8] and the combination of FSI and contact interaction for capturing phenomena such as wet contact or elastohydrodynamic lubrication is discussed in [9] *(Figure 6)*. The coupling of several subdomains with non-matching meshes in computational fluid dynamics can also be efficiently carried out with dual mortar methods, see [10]. This allows to couple very fine boundary layer meshes (e.g. for diffusion layers in an electrochemical bath) to rather coarsely discretized bulk regions without any mesh transition zone.







 $t = 0.42$ 

 $t = 0.95$ 

velocity magnitude  $0.6$ 



#### *Parallel repartitioning and dynamic load balancing*

The presented mortar finite element methods are designed for the use on large cluster systems with many CPUs and distributed memory. An overlapping domain decomposition approach is employed for the parallel distribution of all finite elements in the problem domain. However, the parallel distribution of a mortar interface is not necessarily optimal then. To improve this situation, we introduce an independent parallel repartitioning of all mortar elements at the coupling interface. This rather simple idea allows for perfect parallel scalability within a wide range concerning the number of processors *(Figure 7)*. The proposed procedure can be further refined for unilateral contact applications, where the actual contact zone is not known a priori and may constantly and signifacantly vary over time. Thus, whenever finite deformations and large sliding motions occur, the repartitioning needs to be repeated. Such a dynamic load balancing strategy is typically triggered by a suitable measure for the workload of each individual process. The parallel balance of the workload among all processes is monitored and a simple heuristic criterion whether to apply dynamic load balancing within the current time step or not can be formulated.

#### *Large-scale numerical examples*

The mortar finite element methods presented in this contribution are readily applicable to large-scale simulations of complex processes involving fluid dynamics, structural dynamics or several coupled physical fields. Especially the design of the numerical algorithms as described above, i.e. including parallel repartitioning and dynamic load balancing, assures an excellent parallel scalability when solving very large simulation models with up to several million degrees of freedom. To give an impression of typical problem sizes, snapshots of two large-scale examples from contact dynamics with finite deformations and nonlinear material behavior are shown in *Figure 8*. The finite element mesh for the 3D impact model, for example, consists of 4,255,360 hexahedral elements and 13,994,880 degrees of freedom in total. The numerical solution is performed in parallel on up to 120 cores, using an implicit time stepping scheme and 500 time increments to resolve all contact interactions.

#### *Future trends and challenges*

Although substantial progress towards a truly general purpose mortar finite element framework for computational contact

mechanics or, more general, for non-conforming discretization and interface coupling in complex multiphysics simulations has been made over the last years, there is still room for improvements with regard to several aspects, which were only marginally covered up to now or not addressed at all. This includes smooth interpolation schemes for the mortar coupling surfaces, either through isogeometric formulations based on NURBS or through an adaptation of traditional smoothing procedures to mortarbased formulations. Further extensions towards complex interface effects are also a worthwhile future research direction. This includes anisotropic friction, surface roughness effects, lubricated contact and sophisticated models for surface degradation due to wear. From an algorithmic point of view, the development of tailored linear solvers and preconditioning techniques for the resulting linear systems is currently one of the most important challenges. An out-of-thebox application of highly efficient iterative solvers and preconditioners developed for general solid or fluid mechanics problems (e.g. algebraic multigrid methods) may yield satisfactory results in some cases, but the non-conforming structure of mortar based discretizations precludes an efficient solution in general. In order to tap the full potential of such solution techniques, all available knowledge about the physics and numerics of the underlying problem should be included in the solver design.  $\bullet$ 

#### *Acknowledgements*

We would like to thank our main collaborators at TUM, Prof. M. W. Gee (Mechanics and High Performance Computing) and Prof. B. Wohlmuth (Numerical Mathematics). Also, the help of many current and former members of the Institute for Computational Mechanics is gratefully acknowledged, with special thanks to A. Ehrl, M. Gitterle and T. Klöppel.



#### *Figure 7:*

*Figure 8:*

*two thin-walled tori in 3D (right)*

*Parallel repartitioning and load balancing for a large-scale mesh tying example. The initial partitioning using 32 cores (left) and a strong scaling diagram (right) of the total computation time associated with coupling terms at the mortar interface are illustrated*



#### **References**

- [1] *C. Bernardi, Y. Maday, and A. T. Patera*, **A new nonconforming approach to domain decomposition: the mortar element method**, In H. Brezis and J. Lions (eds.), Nonlinear PDEs and their applications, pages 13–51, Pitman/Wiley: London/ New York, 1994.
- [2] F*. Ben Belgacem*, **The mortar finite element method with Lagrange multipliers**, Numerische Mathematik 84, 173–197, 1999.
- [3] *B. I. Wohlmuth*, **Discretization methods and iterative solvers based on domain decomposition**, Springer-Verlag Berlin Heidelberg, 2001.
- [4] *B. I. Wohlmuth*, **A mortar finite element method using dual spaces for the Lagrange multiplier**, SIAM Journal on Numerical Analysis 38, 989–1012, 2000.
- [5] *A. Popp, M. W. Gee, and W. A. Wall*, **A finite deformation mortar contact formulation using a primal-dual active set strategy**, International Journal for Numerical Methods in Engineering 79, 1354–1391, 2009.
- [6] *A. Popp, M. Gitterle, M. W. Gee, and W. A. Wall*, **A dual mortar approach for 3D finite deformation contact with consistent linearization**, International Journal for Numerical Methods in Engineering 83, 1428–1465, 2010.
- [7] *A. Popp, B. I.Wohlmuth, M. W. Gee, and W. A. Wall*, **Dual quadratic mortar finite element methods for 3D finite deformation contact**, SIAM Journal on Scientific Computing 34, B421–B446, 2012.
- [8] *T. Klöppel, A. Popp, U. Küttler, and W. A. Wall*, **Fluid-structure interaction for nonconforming interfaces based on a dual mortar formulation**, Computer Methods in Applied Mechanics and Engineering 200, 3111–3126, 2011.
- [9] *U. M. Mayer, A. Popp, A. Gerstenberger, and W. A. Wall*, **3D fluid-structure-contact interaction based on a combined XFEM FSI and dual mortar contact approach**, Computational Mechanics 46, 53–67, 2010.
- [10]*A. Ehrl, A. Popp, V. Gravemeier, and W. A. Wall,* **A mortar approach with dual Lagrange multipliers for mesh tying within a variational multiscale method for incompressible flow**, paper in preparation, 2013.

## The Particle Finite Element Method (PFEM) An Effective Numerical Technique for Multidisciplinary Problems in Engineering

*by Eugenio Oñate1 Sergio R. Idelsohn1,2 and Miguel A. Celigueta1 <sup>1</sup> International Center for Numerical Methods in Engineering (CIMNE), Technical University of Catalonia, Barcelona, Spain <sup>2</sup> ICREA Research Professor at CIMNE*

#### *Figure 1:*

*Scheme of a typical solution with PFEM. Sequence of steps for moving a ``cloud'' of nodes representing a domain containing a fluid and a solid part from time n to time n+2*

The analysis of multidisciplinary<br>problems is relevant in many areas of engineering. Examples are common in the study of fluid-soil-structure interaction problems such as the motion of landslides and their effect on reservoirs and adjacent structures, off-shore and harbor structures under large waves, constructions hit by floods and tsunamis, soil erosion and stability of rockfill and earth dams in overspill situations and excavation and drilling problems in civil and oil and gas engineering. Among the many other multidisciplinary engineering problems we note the analysis of multiphase thermal flows, the deformation of material and structures in fire situations and thermal-magnetic-mechanical problems that are found in many industrial forming processes.

The authors and their group have developed in recent years a particular class of Lagrangian formulation for solving multidisciplinary problems involving complex interactions between fluids and solids. The so-called Particle Finite Element Method (PFEM, www.cimne.com/pfem), treats the mesh nodes in the fluid and solid domains as particles which can freely move and even separate from the main



domain representing, for instance, the effect of water drops or soil particles. A mesh connects the nodes discretizing the domain where the governing equations are solved using a stabilized FEM [1-10].

An advantage of the Lagrangian formulation used in the PFEM is that the non-linear and non symmetric convective terms disappear from the fluid equations. The difficulty is however transferred to the problem of adequately (and efficiently) moving the mesh nodes.

#### **The basis of the PFEM**

In the PFEM both the fluid and the solid domains are modelled using an updated *Lagrangian formulation* [2]. That is, all variables are assumed to be known in the *current configuration* at time *t*. The new set of variables in both domains is sought for in the *next or updated configuration* at time  $t + \Delta t$ .

A typical solution with the PFEM involves the following steps:

- 1. The starting point at each time step is the cloud of points in the fluid and solid domains. For instance *<sup>n</sup> C* denotes the cloud at time  $t = t_n$  (Figure 1).
- 2. Identify the boundaries for both the fluid and solid domains defining the analysis domain  $\sqrt[n]{V}$  in the fluid and the solid. This is an essential step as some boundaries (such as the free surface in fluids) may be severely distorted during the solution, including separation and re-entering of nodes. The Alpha Shape method [1,2] is used for the boundary definition.
- 3. Discretize the fluid and solid domains with a finite element mesh  $\mathrm{^{\textit{\prime}}}M.$  We use an effective mesh generation scheme based on an enhanced Delaunay tesselation [1,2]. The quality of the numerical solution depends on the discretization chosen as in the standard FEM. Adaptive mesh refinement techniques can be used to improve the solution. As a general rule for large 3D problems meshing consumes around 15% of the total CPU time per time step in a single processor Pentium IV PC.
- 4. Solve the coupled Lagrangian equations of motion for the overall continuum. Compute the state variables in at the next (updated) configuration for  $t_n + \Delta t$ . velocities, pressure and viscous stresses in the fluid and displacements, stresses and strains in the solid.<br>5. Move the mesh nodes to a new position
- C where  $n + 1$  denotes the time  $t_n + \Delta t$ .
- 6. Go back to step 1 and repeat the solution for the next time step to obtain *n+2C (Figure 1)*.

We emphasize that the key differences between the PFEM and the classical FEM are the identification of the domain boundary and the re-meshing at each time step.

#### **Treatment of contact conditions in the PFEM**

Known velocities at boundaries in the PFEM are prescribed in strong form to the boundary nodes. These nodes might belong to fixed external boundaries or to moving boundaries. Contact between fluid particles and fixed boundaries is accounted for by the incompressibility condition which *naturally prevents fluid nodes to penetrate into the solid boundaries*.

The contact between two solid interfaces is treated by introducing a layer of *contact elements* between the two interacting solid interfaces. This layer is *automatically created during the mesh generation step* by prescribing a minimum distance *(hc)* between two solid boundaries. If the distance exceeds the minimum value *(hc)* then the generated elements are treated as fluid elements. Otherwise the elements are treated as contact elements where a relationship between the tangential and normal forces and the corresponding displacement is introduced *(Figure 2)*. This algorithm allows us to model complex frictional contact conditions between interacting bodies moving in water in a simple manner. The algorithm can also be used effectively to model frictional contact conditions between rigid or elastic solids in structural mechanics applications [9].



#### **Modeling of bed erosion**

Prediction of bed erosion and sediment transport is important in river and environmental engineering. Bed erosion can lead to instabilities of the river basin slopes. It can also undermine the foundation of bridge piles thereby favouring structural failure. Modeling of bed erosion is also relevant for predicting the evolution of surface material dragged in earth dams in overspill situations. Bed erosion is one of the main causes of environmental damage in floods.

The PFEM erosion model [4,8] is based on detaching elements belonging to the bed surface in terms of the frictional work at the surface originated by the shear stresses in the fluid. The resulting erosion model resembles Archard law typically used for modeling abrasive wear in surfaces under frictional contact conditions.

Sediment deposition can be modeled by an inverse process. Hence, a suspended node adjacent to the bed surface with a velocity below a threshold value is attached to the bed surface. Examples of this bed erosion algorithm for modeling excavation and rock cutting problems with PFEM are presented in [9].

#### *Figure 2: Modelling of contact conditions at a solid-solid interface with the PFEM*

*Figure 3: Waves acting on breakwater slopes containing reinforced concrete blocks*



#### *Figure 4a*

*(a) Erosion, transport and deposition of soil particles in a river bed due to an impacting jet stream (b) Erosion of an unprotected shoulder of a breakwater due to sea waves*

#### *Figure 5:*

*Erosion of a soil mass due to sea waves and falling into the sea of an adjacent lorry*





#### **Examples**

#### *Impact of sea waves on piers and breakwaters*

*Figure 3* shows the PFEM analysis of the effect of breaking waves on two different sites of a breakwater in Langosteira harbour (A Coruña, Spain) containing reinforced concrete blocks (each one of 4x4x4 mts).

*Figure 6: Simulation of landslide falling on constructions using PFEM*





#### *Soil erosion problems*

*Figure 4a* shows the capacity of the PFEM

for modelling soil erosion, sediment transport and material deposition in a river bed. The soil particles are detached from the bed surface under the action of the jet stream. Then they are transported by the flow and eventually fall down due to gravity forces into the bed.

*Figure 4b* shows the progressive erosion of the unprotected part of a breakwater slope in the Langosteira harbour under sea waves.



#### *Figure 7:*

*Lituya Bay landslide. (a) Geometry, landslide direction and maximum wave level. (b) Evolution of landslide into the reservoir obtained with PFEM. Maximum level of generated wave (551 mts) in north slope*

*Figure 5* shows the progressive erosion of a soil mass adjacent to the shore due to sea waves and the falling into the sea of an object representing the section of a lorry modelled as a rigid solid.

#### *Modelling of landslides*

The PFEM is particularly suited for modelling landslide motion and its interaction with structures and the environment.

*Figure 6* shows a simulation using PFEM of a soil mass representing a landslide falling on four constructions modelled as rigid body solids.

*Figure 7* shows PFEM results of the 3D analysis of the landslide in Lituya Bay (Alaska) on July 9th 1958. The landslide was originated by an earthquake and movilized 90 millions tons of rocks that fell on the bay originating a large wave that reached a hight on the opposed slope of 524 mts. The maximum water level in north hill obtained with PFEM was 551 mts. The maximum height location differs in 300 mts from the observed value. In the south slope the maximum water height observed was 208 mts, while the PFEM result (not shown here) was 195 mts. [10].

#### *Sinking of ships and collision of ships with ice blocks*

The PFEM can be effectively applied for simulating the sinking of ships under a variety of scenarios. *Figure 8* shows images of the 2D simulation of the sinking of a cargo vessel induced by a breach in the bow region.

*Figure 9* shows an example of the application of PFEM to the study of the collision of a boat with floating ice blocks both modelled as rigid bodies. Indeed, the deformation of the ship structure due to the

> *Figure 10: 2D PFEM analysis of an excavation with a road-header*



ice-ship interaction forces can be accounted for in the analysis.

#### *Excavation and drilling problems*

The PFEM has been successfully applied to the analysis of excavation, dredging and tunneling problems in civil engineering, as well as to drilling and cutting transport problems typical of the oil and gas industry. *Figures 10-12* show some representative examples of this class of problems. For more information see [9].

#### *Simulation of tsunami flow*

*Figure 13* shows a 3D simulation with PFEM of the dragging of cars, barrels and debris in a tsunami flow impacting a vertical wall.

*Figure 8: 2D simulation of the sinking of a vessel. Water velocity pattern at different times during sinking*











*Figure 9: 3D PFEM simulation of a boat colliding with five ice blocks*



*Figure 11:* 

*Simulation of a dredging test with PFEM. Soil particles are suctioned from a cohesive soil mass from the recipient in the right to that in the left*

> *Figure 12: Transport of drill cuttings in mud within a curved borehole pipe with rotational annulus*





*Behaviour of object in fire situation* The PFEM has been effectively applied to the simulation of burning, melting and dripping of object in fire situations. *Figure 14* shows the PFEM simulation of the melting

and dripping and polymer layer protecting three cables. *Figure 15* shows three instants of the burning, melting and dripping of a thermoplastic object in a close cavity. For more information see [7,11].  $\bullet$ 







#### *Figure 14:*

*PFEM simulation of the melting and dripping of a polymer layer protecting three cables. Figures show the evolution of the 4-noded tetrahedra mesh discretizing the polymer*

*Figure 15:* 

*PFEM analysis of the evolution of the burning, melting and dripping of a rectangular thermoplastic object in a closed cavity*







#### **References**

- [1] *Idelsohn, S.R., Oñate, E. & Del Pin, F.*, **The particle finite element method: a powerful tool to solve incompressible flows with free-surfaces and breaking waves**, Int. J. Num. Meth. Engng,. 61, pp. 964-989, 2004.
- [2] *Oñate, E., Idelsohn, S.R., Del Pin, F. & Aubry, R.,* **The particle finite element method. An overview**, Int. J. Comput. Methods, 1(2), pp. 267-307, 2004b.
- [3] *Idelsohn, S.R., Oñate, E., Del Pin, F. & Calvo, N.*, **Fluid-structure interaction using the particle finite element method**, Comput. Meth. Appl. Mech. Engng., 195, pp. 2100-2113, 2006.
- [4] *Oñate, E., Celigueta, M.A. & Idelsohn, S.R.*, **Modeling bed erosion in free surface flows by the Particle Finite Element Method**, Acta Geotechnia, 1(4), 237-252, 2006.
- [5] *Larese, A., Rossi, R., Oñate, E. & Idelsohn, S.R.*, **Validation of the Particle Finite Element Method for free surface flows**, Engng. Computations, 25(4), pp. 385-425, 2008.
- [6] *Idelsohn, S.R., Mier-Torrecilla, M. & Oñate, E.*, **Multi-fluid flows with the Particle Finite Element Method**, Comput Methods Appl Mech Engrg., 198, pp. 2750-2767, 2009.
- [7] *Oñate, E., Rossi, R., Idelsohn, S.R. & Butler, K.*, **Melting and spread of polymers in fire with the Particle Finite Element Method**, Int. J. Numerical Methods in Engng., 81(8), 1046-1072, 2010.
- [8] *Oñate, E., Celigueta, M.A., Idelsohn, S.R., Salazar, F. & Suárez B.*, **Possibilities of the Particle Finite Element Method for fluid–soil–structure interaction problems,** Comput. Mech., 48, pp. 307-318, 2012.
- [9] *Carbonell, J.M,. Oñate, E. & Suárez, B.*, **Modelling of tunnelling processes and cutting tool wear with the Particle Finite Element Method**, Computational Mechanics, Vol 1, 2013.
- [10] *Oñate, E., Salazar, F. & Morán, R.*, **Modeling of landslides into reservoir with the Particle Finite Element Method**, Research Report CIMNE PI355. Submitted to Int. J. Numerical Methods in Geomechanics, 2013.
- [11] *Oñate, E., Marti, J., Ryzhakov, P., Rossi & R., Idelshon, S.R.*, **Analysis of the melting, burning and flame spread of polymers with the Particle Finite Element Method**. Submitted to Computer Assisted Methods in Engineering and Science (CAMES), 2013.

## $MULTIGRID TECHNIQU<sub>2</sub>$ 1984 GUIDE WITH APPLICATIONS TO FLUID DUNAMICS, REVISED EDITION

*Achi Brandt and Oren E. Livne Brandt and Oren E. Livne SIAM, Philadelphia, USA, 2011*

B

O

O

K

R

E

V

I

E

W



#### *ISBN: 978-1611970746*

*218 pages, paper cover, \$79.00 (List Price).* 

*Contents: Preface; Chapter 0: Introduction; Chapter 1: Elementary Acquaintance with Multigrid; Chapter 2: Stable Discretization; Chapter 3: Interior Relaxation and Smoothing Factors; Chapter 4: Interior Two-Level Cycles; Chapter 5: Boundary Conditions and Two-Level Cycling; Chapter 6: Many-Level Cycles; Chapter 7: Full Multi-Grid (FMG) Algorithms; Chapter 8: Full Approximation Scheme (FAS) and Applications; Chapter 9: Local Refinements and Grid Adaptation; Chapter 10: Higher-Order Techniques; Chapter 11: Coarsening Guided By Discretization; Chapter 12: True Role of Relaxation; Chapter 13: Dealgebraization of Multigrid; Chapter 14: Practical Role of Rigorous Analysis and Quantitative Predictions; Chapter 15: Chains of Problems. Frozen τ; Chapter 16: Time Dependent Problems; Chapter 17: Cauchy-Riemann Equations; Chapter 18: Steady-State Stokes Equations; Chapter 19: Steady-State Incompressible Navier-Stokes Equations; Chapter 20: Compressible Navier-Stokes and Euler Equations; Chapter 21: Remarks on Solvers for Transonic Potential Equations; Appendix: Test Cycle: MATLAB Code; Bibliography; Index..*

This is a new edition of the successful guide to multigrid (MG) techniques that the first author published in 1984. In turn, the 1984 guide was originally based on the notes of the first author, who was one of the main inventors of the MG method, with his groundbreaking 1973 paper introducing the method and the many important extensions he has published later on with his group. The second author has been a member of that group. In the Preface, the authors state that the new edition is not essentially different than the 1984 one, and that only few essential modifications were made. As a consequence, this guide is not fully updated, and falls short of representing later MG developments. The authors are working on a Multigrid Guide 2.0 book that will be up to date when published.

For the readers of this review, an explanation of the basic idea underlying the MG method can be found in the article "More CM Questions of the Month" appearing in the present IACM Expressions issue. This basis of MG is presented only very briefly in the Brandt-Livne book, since the authors assume that the reader is already familiar with it. As Section 0.2 explains, the book is intended for readers who have been exposed to the basics of MG, but would like to understand the method in depth, to be able to implement the method in a good way and to identify and correct bugs that cause the deterioration of the optimal performance of the method. This last point is crucial, since in many cases, by not implementing the method properly one obtains a code which yields sub-optimal results that are still converging and are better than those obtained with a single uniform grid. As the authors write on p. 3: "It is important to work in that spirit: Do not just observe what efficiency is obtained by a given MG algorithm, but ask yourself what is the ideal efficiency and find out how to obtain it." The book includes a large collection of important tips that are all geared toward obtaining optimal performance out of a MG code.

*by* DAN GIVOLI *Technion — Israel Institute of Technology* givolid@aerodyne.technion.ac.il



*Achi Brandt Oren Livne* 





Chapter 0 also delightfully presents the "philosophy" of multi-level methods, which can be summarized by the "golden rule" (p. 1): "The amount of computational work should be proportional to the amount of real physical changes in the computed system. Stalling numerical processes must be wrong." The authors provide a few examples to this rule, including the example of iterative processes for solving algebraic equations arising from discretizing PDEs, in which little progress toward the exact solution is made from one iteration to the next. Then the authors discuss the benefits of using MG methods for the solution of various types of problems. This "philosophical" spirit lingers on throughout the book, raises it beyond the technical level, and gives it an interesting and thought provoking flavor.



The book consists of a preliminary part and three main parts. The preliminary part (Chapters 0 and 1) covers, in addition to the philosophy of multi-level methods, a brief elementary introduction to MG. Part I (Chapters 2-7) discusses step by step the ingredients of the MG method, from the formulation of good discretization schemes up to Full MultiGrid (FMG) algorithms. The structure of FMG with one V-cycle per level is illustrated in *Figure 1* which is taken from the book. To ensure optimal performance, each of the ingredients of MG must be implemented correctly. Part II (Chapters 8-16) covers more advanced problems, techniques and insights, and discusses various improvements to the basic MG. Part III (Chapters 17- 21) includes applications of MG in fluid dynamics. Appendix A inclues a MATLAB code, implementing the MG cycle for the Poisson equation in a rectangle. This code and its results are discussed in Section 1.5. The reader can experiment with the code, to gain deeper understanding of the MG concepts. Most of the book relates to linear elliptic boundary value problems, but certain sections discuss time-dependent problems and nonlinear problems.

*Full MultiGrid (FMG) algorithm with one V-cycle per level. This figure appears in the book as Fig. 1.2 on p. 19*

Figure 1: The notation used here is partly different than that usually used in the CM literature, but one may get used to it quickly. The error is denoted by v (not by e). There is no index for iteration number; instead the solution in the last iteration is denoted  $\tilde{u}$  or  $\tilde{u}^h$ , and the solution in the new iteration is denoted  $\bar{u}$  or  $\bar{u}$ <sup>h</sup>. The error in the last iteration is denoted v or v<sup>h</sup> (without a tilde, which is slightly confusing).

> Many of the explanations found in this book are heuristic, and many of the tips are described in general terms. There is much more text than equations. Different authors have different writing styles, and perhaps some readers would prefer more equations and a more concrete demonstration of the concepts. As for myself, I find the writing style effective, in that it produces a highly interesting reading material (some segments are not less than fascinating), and does not plunge into too many technical details.

> I will mention a few minor deficiencies that caught my eye. First and foremost, the index misses many entries and could have been much fuller and more helpful. For example, on p. 10 the authors write "An important quantity therefore is the *convergence factor* ..." (the italics appear in the original text). If this quantity is important, how come "convergence factor" does not appear in the index? In fact, "convergence" is not indexed at all. The same is true regarding "amplification factor", "V-cycle", "algebraic MG" and many other essential terms used (and italicized) in the text. This is a pity, since a good index is essential for an optimal use of a reference book.

Second, the MG code given in Appendix A is quite basic and is introduced in Section 1.5 of the preliminery part of the book. The code is not referred to again in any of the sections in Parts I-III. It would have been nice if the code included some of the more advanced features discussed in this book, and the text pointed to the code throughout the discussion to demonstrate the various technical aspects of the issues discussed.

Also, the example output of the code appearing on pp. 16-17 includes a column of numbers entitled "Error Norm", and after each cycle the "convergence factor" is printed. The latter is defined in eq. (1.5) as the ratio between the errors in two consecutive relaxation sweeps. However, a look at the code itself in Appendix A reveals that the routine *errornorm* computes the norm of the *residual* and not that of the error. (No exact solution is available and so the error is not known.) The difference between the concepts "error" and "residual" is significant, and a book on MG should avoid mixing between them.

I will slightly elaborate on some of the chapters of Part II which I personally found to be the most interesting in the book. Chapter 8 discusses the probably most important method that goes beyond classical MG: the Full Approximation Scheme (FAS). The difference between FAS and MG is in the coarse grid correction step; in FAS an additional term is included in the coarse-grid equation, which represents a correction to this equation designed to make its solution coincide with the fine-grid solution. The authors explain the advantages of FAS, especially but not exclusively to nonlinear problems, and recommend that it always be preferred over classical MG. Chapter 9 discusses local grid refinement and adaptation. *Figure 2* is taken from this chapter, and shows sets of rotated cartesian grids around an interior thin layer. Chapter 10 talks about high-order techniques, including the very interesting idea of double discretization. Chapters 11 and 12 are "free discussions" with interesting comments on coarsening and relaxation.



*Figure 2: Grid orientation around an interior thin layer. This figure appears in the book as Fig. 9.3 on p. 105*

Chapter 13 is entitled "Dealgebraization of MG" but is in fact divided into two: in the first part MG is viewed as a method applied to the original PDE, and thus is disconnected from the pure algebra, whereas in the second part the authors briefly discuss Algebraic MG, which was just a trend in 1984, and since then has developed a lot. This latter discussion is of course very outdated. Chapter 14 is a collection of views, a few of them somewhat provocative, about the role of rigorous analysis and of quantitative predictions of convergence rates. The conclusion at the end of Section 14.1 would surprise many: "In sum, for all its pure-mathematical interest and intelectual challenge, much of the existing rigorous approach is not a practical tool. It has played no significant role in developing the various algorithms and insights described in this book. Its only role has generally been to enhance our confidence in the method, a psychological role that should not be slighted." Regardless of whether I agree or not with this point of view, I find Chapter 14 to be extremely interesting and refreshing.

In summary, while this should probably not be the first source that one reads about Multigrid, since it assumes familiarity of the reader with the basic method, it is certainly an excellent second source on advanced MG methods, especially for readers who wish to exploit the method to its utmost potential.  $\bullet$ 

# More CM Questions of the Month

*by Dan Givoli Technion, Israel givolid@aerodyne. technion.ac.il* This is the second part of an article that appeared in IACM Expressions No. 31,<br>June 2012. Here is a short reminder of what the CM Questions of the Month are.

During the last four years, the author of this article has been editing an electronic newsletter on Computational Mechanics (CM), distributed twice a month to more than 400 subscribers who constitute the Israeli CM community (about 50 of them are full members of the Israel Association for Computational Methods in Mechanics – IACMM). This newsletter includes a section called "The Question of the Month," that is a riddle on CM subjects which the readers are asked to solve. Each month the answer to the Question of last month is published, along with the names of those readers who answered it correctly, and a new Question is posed. Sometimes interesting discussions develop, as readers comment on the Questions and on the answers.

The Questions, which span all areas of CM, are composed with an educational goal in mind. Some of the questions may be trivial to some of the readers, who have different backgrounds in industry and academia, but hopefully there is always something new to learn. Sometimes the Questions are quite theoretical, while occasionally they are very practical. Some of the readers who frequently send me their answers and comments are internationally distinguished researchers (like Achi Brandt, Roland Glowinski, Rafi Haftka and Eli Turkel to name just a few; there are others but I will stop here in fear that I will forget someone). Their participation in the discussion on the Questions is an important contribution to the educational benefit of this "game", and encourages other members of the community to participate as well.

IACM Expressions No. 31 included a first collection of Questions, their Answers, and in some cases comments that were made on them by readers. Here we present a second collection. In order to give you, the reader of this article, a chance to think about the Questions before looking at their answers, we first write down all the selected questions, and only then their associated answers and comments.

#### *Question 1:* **The October 2010 Question of the Month: Benefit of Coarse Meshes**

The following situation is typical. We construct a model and run it with a certain grid/mesh, and get results that turn out not to be accurate enough. Then we realize that our grid was too coarse, and we "correct" the situation by using a finer grid.

Now, there is a known method in which *a coarse grid* is used to "correct" (in some sense) *the fine-grid* solution. What is this method, and how does this "correction" work?

*Peter Lax (left) and Burt Wendroff* 



#### *Question 2:* **The September 2011 Question of the Month: Dissipative Schemes**

Various time-depenednt problems in mechanics have the property that energy is preserved. Of course, if one introduces damping or another dissipative mechanism into the problem there is no preservation of energy, but in many cases people do want to look at models that have no damping in them.



*Energy Conserving Swimming*



*Dissipative Swimming*

Now, there are numerical methods that are energy-preserving. So, if we use such a method to solve a problem whose exact solution preserves energy, the energy-preservation property will be inherited by the approximate solution.

This sounds great. So why do people sometimes prefer to use a dissipative method, e.g., the Lax-Wendroff scheme, instead of an energy-preserving method, even if they know that the exact solution *is* energy preserving?

> **j=INT(m/(N-2)) i=m-j\*(N-2) k=i+3+j\*N**

#### *Question 3:* **The January 2012 Question of the Month: Parallel Code**

This Question was designed mainly by Jonathan Tal. It requires light programing skills. **Do m = 0, N\*(N-2)-1**

Consider the following loop (right) taken from a pseudo-code that implements some algorithm:

Assume that the number N is very large, say N<sup>2</sup> is a few millions, and therefore this loop entails "heavy" computing. The function INT(...) takes the integer value of a number. For example, INT(3.9)=3 . **Enddo**

The question is: Does this loop lend itself to parallel computing, namely to the use of a computer with many processors that can work in parallel? If the answer is yes, please explain how "the work" done in this loop can be divided among the various processors. If the answer is no, please explain why not. In that case, think about a way to write this piece of code differently so as to make it amenable to parallelization.

(Hint: if the algorithm is too abstract, try N=5.)

#### *Question 4:* **The September 2012 Question of the Month: Instabilities in Formulations of Elliptic Problems**

The following question is dedicated to the memory of my old-time Brazilian friend Prof. Leo Franca who passed away this month. Leo was a great researcher who has made important contributions to CM, especially in the area of stabilization techniques.

Many of us know that a convergent numerical method must be:

(1) locally accurate,

(2) stable.

This is what the famous Lax theorem tells us. In time-dependent problems, the lack of stability usually manifests itself in that the solution "blows up" in time. Namely, at a certain time the solution begins to grow (typically exponentially fast) in an unbounded way. For example, this happens when one uses explicit time-marching with a time-step which is not small enough (thus violating the so-called CFL condition).

However, consider now a steady-state or static problem (in mathematical terms an elliptic problem), where time is not involved at all. Let us assume that the numerical method that we use gives us a non-singular system of algebraic equations that can be solved. And suppose the method can be shown to be locally accurate.

Can the method be unstable under such circumstances? If it can, how would the instability manifest itself in the solution? The solution cannot "blow up in time", because there is no time in this problem. Give at least one example for an instability in the steady-state or static case, and explain how the instability is "seen".

*Leopoldo (Leo) Franca (1959-2012)*







**v(k) = v(k-1) \* const1 + v(k-2) \* const2**







*Parallel computing*



#### *Answer to question 1:* **Benefit of Coarse Meshes**

What I had in mind when asking this question was multigrid methods. The main inventor of multigrid was Prof. Achi Brandt from the Weizmann Institute, whom we are very proud to have as a member in our community. A very rough description of the basic idea of multigrid is as follows.



*Initial error, before Gauss-Siedel iterations are performed.*



*Error obtained after a number of Gauss-Seidel iterations.*



*The smooth error on the fine grid (blue) turns into an oscillatory error (green) on the coarse grid*.





*Achi Brandt*

iterative method, it is the smooth (i.e., slowly varying) modes in the error that are difficult to control, and may require a huge number of iterations to decay. Now, a crucial point that is the basis for multigrid is that what is considered a "smooth" mode or an "oscillatory" mode depends on the grid/mesh density. A function may be claimed to be slowly varying (smooth) if it is "seen" through a fine grid, but it may be regarded as oscillatory when "seen" through a coarse grid! Multigrid methods exploit this fact by making use of a coarse grid, or actually a hierarchy of coarse grids, that cause (in a way that we shall not go into here) the fast decay of those modes that are slowly-varying on the fine grid. The operation that is associated with this is called "coarse-grid correction" which connects to our Question.

I strongly recommend the book "A Multigrid Tutorial" of W.L. Briggs to anyone who wants to learn about multigrid for the first time. I think it is a wonderful book.

Some readers (RG, RH, ET) mentioned also other methods which make use of a coarse grid to "correct" a numerical solution. One such method is Richardson's Extrapolation. I will not describe it here since a short time ago it was described very nicely by Micha Wolfshtein in his comment on a previous Question of the Month. Yet another class of methods that "corrects" the solution via a coarse grid is called Deferred Corrections; see, e.g., the paper by Rangan from the Courant Institute in **http://www.cims.nyu.edu/~rangan/sdcdae\_BIT.pdf.**



*Micha Wolfshtein*



*Lewis F. Richardson (1881-1953)*



*Aaditya V. Rangan*

One reader (ZZ) pointed out that there were pathological cases, usually associated with some kind of singularity, in which the numerical solution behaves *worse* as the mesh is refined beyond a certain level. In simple words, the solution does not converge as the mesh is refined; yet the solution obtained with a "reasonably" coarse mesh is useful to engineering practice. There are a number of well-known examples of this scenario, like concentrated loads in certain configurations, shear bands when analyzed with standard FE methods, etc.

*Correct answers were obtained from: Orna Agmon Ben-Yehuda, Rafi Haftka, Amiel Herszage, Roland Glowinski, Stephane Seror, Eli Turkel, Asher Yahalom, Zvi Zaphir.*





![](_page_25_Picture_26.jpeg)

*Roland Glowinski and a friend Amiel Herszage Eli Turkel Rafi Haftka (Prof. Glowinski is a foreign full member of IACMM.)*

![](_page_25_Picture_28.jpeg)

#### *Answer to question 2:* **Dissipative Schemes**

There are a number of reasons (somewhat related to each other) for sometimes preferring a dissipative scheme over an energy-preserving one:

- **\*** Dissipative schemes typically have better stability properties than non-dissipative schemes. There are known cases where a certain discrete time-dependent model, based on a standard energy-preserving scheme, is unstable (and the solution blows up exponentially in time), but the replacement of the scheme with a dissipative scheme cures the instability.
- \* Using a dissipative scheme instead of an energy-preserving scheme is sometimes equivalent to introducing artificial damping/viscosity/dissipation into the problem. This often makes the problem more "well behaved" for numerical treatment. For example, suppose the exact solution of the original problem involves a sharp shock. With standard numerical methods it is very difficult to capture the shock, and in many cases the appearance of the shock may lead to a serious deterioration of the entire numerical solution. By introducing artificial viscosity (via the use of a dissipative scheme), the shock is slightly smeared, and this typically results in a much better behavior of the numerical method. The "trick" of a good dissipative scheme is that it achieves this without (significantly) damaging the accuracy of the solution.
- **\*** Some dissipative schemes are designed so that they selectively damp away "components" of the solution that are undesired. For example, numerical solutions of wave problems include "modes" of various frequencies, and whereas the low-frequency modes are usually well resolved, the high-frequency modes predicted by the method are totally spurious. These high spurious modes may cause a lot of trouble, and smart dissipative schemes suppress them while leaving the low modes unharmed.
- **\*** AY suggested: if one is looking for a steady state solution by advancing the solution in time, one may wish to use a dissipative scheme in order to converge to the steady state smoothly and avoid ever-lasting oscillations.
- **\*** ET and AH also gave more specific explanations on the reason that the Lax-Wendroff scheme is successful. I will not include them here for the sake of brevity.
- **\*** ET has made a very interesting "cultural" observation. He writes that in some fields like meteorology (numerical weather prediction), practitioners often refuse to use dissipative schemes, since these schemes "reduce the mass of the atmosphere", which the practitioners consider inappropriate. In other words, some or most computational meteorologists insist on looking at the problem in a very physical way, and so they view dissipative schemes as something that contradicts the laws of nature. I will leave it to you to decide if this approach is justified or helpful.

![](_page_26_Picture_8.jpeg)

*Correct answers were obtained from:* Orna Agmon Ben-Yehuda, Michael Bogomolny, Roland Glowinski, Amiel Herszage, Oren Livne, Eli Turkel, Asher Yahalom.

![](_page_26_Picture_10.jpeg)

*Oren Livne*

![](_page_26_Picture_12.jpeg)

*Orna Agmon Ben-Yehuda* 

#### *Answer to question 3:* **Parallel Code**

The loop does not lend itself directly to parallel computing (at least at first sight) since there are dependencies between the entries of the vector v. Since every v(k) depends on v(k-1) and v(k-2) we cannot let different processors compute different groups of these entries, because each processor would need information from the other processors.

However, not all is lost. To understand what is going on exactly in this loop, let us look at the case N=5. For N=5, the loop's parameter m goes from 0 to 14. The corresponding values of j are:

 $j = 0, 0, 0, 1, 1, 1, 2, 2, 2, 3, 3, 3, 4, 4, 4.$ 

The corresponding values of i are:

 $i = 0, 1, 2, 0, 1, 2, 0, 1, 2, 0, 1, 2, 0, 1, 2.$ 

The corresponding values of k are:

k = 3, 4, 5, 8, 9, 10, 13, 14, 15, 18, 19, 20, 23, 24, 25.

Since every  $v(k)$  depends only on the two predecessors  $v(k-1)$  and  $v(k-2)$ , we see that there is a separation into groups here, after all. For example, v(8), v(9) and v(10) do not depend on  $v(3)$ ,  $v(4)$  and  $v(5)$ , but depend only on  $v(6)$  and  $v(7)$  that do not appear at all in this loop! (Their values were read or calculated somewhere earlier in the program.) Therefore, the processor calculating  $v(8)$ ,  $v(9)$  and  $v(10)$  can be different than the processor calculating  $v(3)$ ,  $v(4)$  and  $v(5)$  – there is no dependency between these two groups.

*Rachel Gordon* 

![](_page_27_Picture_10.jpeg)

More generally, groups of size N-2 are created in this loop, and these groups can be assigned to different processors and can be computed independently of each other. A clear way to implement this is to notice that the given loop is equivalent to the following one:

**Do j = 0, N-1 Do i = 0, N-3 v(i,j) = v(i-1, j) \* const1 + v(i-2, j) \* const2 Enddo**

Here we replaced the vector  $v(k)$  by a matrix  $v(i,j)$ . Clearly, we see that while  $v(i,j)$ depends on previous i's it does not depend on previous j's. Therefore, we can assign different values of j to different processors.

**Correct answers were obtained from:** Ran Ganel, Rachel Gordon.

#### *Answer to question 4:* **Instabilities in Formulations of Elliptic Problems**

Here are a few examples for an instability appearing in static / steady-state cases.

1. AH and RBZ give an example of a finite difference scheme for steady-state incompressible flow problems. If the difference scheme is not appropriate, the pressure may strongly oscillate from one grid point to another (or from one cell to

> another in finite volume methods). This is called "checkerboard pattern," because in extreme cases one would get a change of sign between neighboring cells, which reminds one of the black and white cells on a checkerboard. One possible remedy in this case is to use what is called a staggered grid.

*Checkerboard Chekcerboard pattern*

- 2. A similar situation happens in "mixed finite element" methods. If one does not use appropriate shape functions for the various variables involved, an instability may arise in the form of a "checkerboard pattern". There is a condition (called the Babuska-Brezzi condition) for stability, and if the shape functions satisfy this condition then they are safe for use.
- 3. Another instability phenomenon which may arise in mixed finite element methods, if one does not use appropriate shape functions, is called "locking". In this case, the solution is not oscillatory but simply approaches zero (instead of approaching the exact solution) This can be explained in the following manner. Mixed finite element methods try to enforce some governing equations (say the momentum equations) and also a constraint (say the incompressibility constraint). If the approximation space is not chosen well, the constraint may be enforced too strongly so as to dominate the entire system of equations. Good approximation gives good balance between the governing equations and the constraint.
- 4. RBZ: "In solid mechanics, the so-called "hourglass modes" are kinematic patterns of single cells/elements deforming rectangles into trapezoid with no stress involved when a constant stress is assumed within the cell/element. These modes are manifested as zigzag global deformation patterns. They are avoided by either higher order scheme, higher integration order within elements or by adding a small suppressing anti-hourglass artificial viscosity term."

![](_page_28_Picture_3.jpeg)

- 6. OABY gives an example of a method for mesh smoothing. This in fact involves the solution of Laplace's equation. "In most smoothing methods, we more or less move each vertex to the center of its neighbours, for example according to a rule that says that each edge is a spring, so that the springs dictate the direction and amount of motion." If one takes too large steps in this process, one may get an entangled mesh, which becomes worse and worse with further steps. (Is this an instability? Probably yes, because by definition an instability is a situation where small changes in the data cause large changes in the solution, and this seems to be the situation here.)
- 7. In a static problem involving a very thin boundary layer (e.g., a string on an elastic foundation with a very stiff elastic constant), if one does not treat the boundary layer appropriately, one would get spurious oscillations in large parts of the domain (far beyond the boundary layer itself). This is essentially a stability problem.
- 8. If the solution of a steady-state problem involves a discontinuity, or a shock, and it is not appropriately treated, again one would get spurious oscillations in large parts of the domain

**Correct answers were obtained from:** Orna Agmon Ben-Yehuda, Rami Ben-Zvi, Amiel Herszage, Oren Livne.

![](_page_28_Picture_8.jpeg)

*Hourglass Hourglass mode*

*Rami Ben-Zvi*

![](_page_29_Picture_0.jpeg)

for all inclusions under **JSCES** please contact **Kenjiro Terada** tei@irides.tohoku.ac.jp

Figure 1: Special lecture by Professor Toshiaki Hisada in the JSCES Symposium

![](_page_29_Picture_3.jpeg)

#### Figure 2:

Group shot of some JSCES's executive council members and recipients of The JSCES Award, Kawai Medal, Shoji Medal, **Technical Prize. Outstanding Paper Award** and **Young Researcher Award** 

#### The Japan Society for Computational Engineering and Science

#### **General Assembly Meeting Assembly Meeting**

he fourth assembly meeting of the JSCES, which was registered as a general incorporated organization, was held on May 16th, 2013. The hot topic of the meeting was the revision of Article 6 in Chapter 2, which establishes the "kinds of constituent members and their rights" in the JSCES's bylaw, which strictly follows the Act on General Incorporated Associations and General Incorporated Foundations. The point was the differentiation the representative members that should be the organization staffs covered in law from the regular members; see the JECES's website at http://www.jsces.org/e/Overview/article.html for the details.

Prior to the deliberation in the assembly, a special lecture was presented by Professor Toshiaki Hisada of The University of Tokyo. The topic was the "Multiscale Multiphysics Heart Simulator" that he has been developing for more than a decade. *(Figure 1)*.

### *Award Ceremony for JSCES Prizes: Award Ceremony for JSCES Prizes:*

After the meeting, we had the award ceremony for awarding JSCES prizes to senior and young researchers and practitioners. This year's recipients are Prof. Noboru Kikuchi (The JSCES Grand Prize), Prof. Y. Tomita (The JSCES Award) and Prof. F. Kikuchi (The JSCES Award), Prof. N. Takano (Kawai Medal), Dr. N. Sasaki (Shoji Medal). Paper awards associated with the Transaction of the JSCES (see, https://www.jstage.jst.go.jp/browse/jsces) were also given the following researchers: Dr. N. Onodera, Prof. T. Aoki, Mr. K. Sugiura (Outstanding Paper Award), Dr. K. Murotani, Dr. M. Daichi, Dr. T. Fujisawa, Prof. S. Koshizuka and Prof. S. Yoshimura (Outstanding Paper Award), Dr. H. Doi, Dr. L. Yinsheng and Dr. H. Nakamura (Technical Prize), Dr. H. Akiba, Prof. S. Yoshimura and Mr. Y. Shibata (Technical Prize), Prof. A. Santo (Young Researcher Award), Prof. M. Fujikawa (Young Researcher Award). Moreover, Prof. H. Ohtsubo, Prof. S. Kobayashi and Prof. N. Tosaka were awarded as honorary members *(Figure 2)*.

The JSCES, which has about 850 IACM members, is directing various international activities as an IACM affiliated society in Japan, promotes exchanges in individual associations and societies on computational mechanics. The JSCES is now planning to host the International Conference on Computational Engineering and Science for Safety and Environmental Problems (COMPSAFE 2014) in Sendai, Japan, April 13-15, 2014 as a special interest conference of IACM and a thematic conference of APACM, which will be co-organized with the Japan Association for Computational Mechanics (JACM) and International Research Institute of Disaster Science, Tohoku University; see the conference webpage at http://www.compsafe2014.org/ $\bullet$ 

![](_page_29_Picture_13.jpeg)

## **USACM**

## **USACM Workshop on Nonlocal Damage & Failure Peridynamics and Other Nonlocal Models** March 11-12, 2013, San Antonio, Texas

USACM sponsored, along with SiVRiT, the "Workshop on Nonlocal Damage and Failure: Peridynamics and Other Nonlocal Models". The Workshop was held on the University of Texas at San Antonio Downtown Campus, March 11-12, 2013 and organized by Professors John Foster (UT-San Antonio), Florin Bobaru (University of Nebraska-Lincoln), Philippe Geubelle (University of Illinois at Urbana-Champaign) and Dr. Stewart A. Silling (Sandia National Laboratories). It was co-sponsored by the UTSA Center for Simulation Visualization and Real-Time Prediction (SiViRT), Prof. Yusheng Feng, Director.

An opening reception was held at the Doubletree Hotel across the street from the campus the evening prior. The workshop was attended by 40 participants and featured 25 talks in a single session format over two days focusing on the following topics:

- The need for nonlocal modeling
- Nonlocal models in dynamic brittle fracture, plasticity, visco-elasticity, fiber-reinforced composites, multiphysics problems and extreme conditions (high-velocity impact, fragmentation)
- Multiscale modeling and adaptivity in nonlocal models
- Numerical methods and analysis for nonlocal models
- Nonlocal calculus and mathematical analysis of nonlocal/peridynamic models
- Software implementations of nonlocal models
- Connections between different nonlocal models

The Workshop featured ample times for discussion throughout the program, during workshop lunches, and the conference dinner, which was held at Mi Tierra Restaurant on Monday evening. Participants from applied mathematics, modeling, and computations communities, as well as from industry, generated questions and offered diverse view-points and comments which would not have been possible in a different meeting format. One-on-one discussions during the breaks, and special "end-of-the-day" discussion sessions were extremely appreciated by the participants. A plan for "what's next" and observations on challenges and opportunities in nonlocal modeling of damage and failure, were formulated. These included uploading presentations on the web, and work on an edited volume on peridynamics with contributions from the workshop participants. Participants expressed interest in meeting again in 2015. More information about the workshop can be found at **http://ndf2013.usacm.org/. ●** 

> *Figure 2: Participants at the workshop dinner*

*for all inclusions under USACM please contact* **info@usacm.org**

*Figure 1: Dr. Stewart Silling discussing peridynamics concepts with two graduate student participants*

![](_page_30_Picture_15.jpeg)

![](_page_30_Picture_16.jpeg)

## *USACM Upcoming Events USACM Upcoming Events*

- m **12th U.S. National Congress on Computational Mechanics**, July 22-25, 2013, Raleigh, North Carolina (http://12.usnccm.org)
- m **ICES/USACM Workshop on Minimum Residual and Least Squares Finite Element Methods**, November 4-6, 2013, Austin, Texas (https://sites.google.com/site/workshoplmr/)
- m **Multiscale Methods and Validation in Medicine and Biology II: Biomechanics and Mechanobiology**, February 13-14, 2014, Berkeley, California (http://mmvmb2.usacm.org)

# ACM 2013 - A Conference Celebrating

*by Y. Bazilevs, K. Takizawa & T.E. Tezduyar*

**A**Conference Celebrating the 70th Birthday of<br>Thomas J.R. Hughes was held on February 24–27, 2013 in San Diego, California. Yuri Bazilevs (UC, San Diego), Kenji Takizawa (Waseda University) and Tayfun Tezduyar (Rice University) were the conference co-chairs. The 17th International Conference on Finite Elements in Flow Problems (FEF 2013) was a special track within the birthday celebration conference. Over 400 people attended the birthday conference, and over 350 presentations comprised the conference technical program, resulting in three days of intense, high-quality exchange of the latest ideas, trends, and results in many areas of computational mechanics. One of the co-chairs, in the closing remarks at the banquet, spoke of the event as: "The high energy level reached at the welcoming reception on Sunday was maintained for the duration of the conference."

![](_page_31_Picture_3.jpeg)

*Figure 1: Conference programme* 

ACM 2013 was unusual in that it had a dual objective. On the one hand, it was a celebratory conference, in which the participants honored Thomas Hughes and recognized his numerous, important, and sustained contributions to computational mechanics.

![](_page_31_Picture_6.jpeg)

On the other hand, ACM 2013 included FEF 2013, which has been a standalone conference series for many years, with the main objective to provide a venue for the exchange of ideas and latest research results in finite element and related techniques for applications involving fluid mechanics and transport phenomena. Making FEF 2013 a large part of the birthday celebration conference was a way for the community to honor Thomas Hughes for his contributions to the development of finite element methods for fluid mechanics.

![](_page_31_Picture_8.jpeg)

*Figure 3: Conference banquet*

One of the highlights of ACM 2013 was a two-day short course on Computational Fluid–Structure Interaction (CFSI) taught by the conference co-chairs. The short course preceded the conference and attracted about 40 participants, ranging from masters students to chaired professors.

# the 70th Birthday of Thomas J.R. Hughes

![](_page_32_Picture_1.jpeg)

The course struck a good balance between topics that are now considered classical, and those just appearing in archival research journals. Many of the short-course

participants had copies of the just-published CFSI textbook co-authored by the short-course lecturers (Y. Bazilevs, K. Takizawa and T.E. Tezduyar, "Computational Fluid–Structure Interaction. Methods and Applications", Wiley 2013), and the book is expected to further enhance the learning experience of the participants of the future CFSI short courses.

![](_page_32_Picture_4.jpeg)

*Figure 4: Participants of the CFSI short-course during a break*

*Figure 5: CFSI short-course lecturers: K. Takizawa, Y. Bazilevs, and T.E. Tezduyar*

The efforts of many contributed to the overall success of the event. Participants traveled from far away places to attend the conference. Minisymposia organizers made a careful selection of the speakers, and put together presentation lineups that were combined into an impressive technical program. Semi-plenary lecturers and keynote speakers, all highly visible researchers recognized worldwide for their achievements, delivered stimulating presentations. Cristina Forace and Angel Priegue of the CIMNE Congress Management

Department did a laudable job in setting up the conference Website and registration system. Ruth Hengst of ICES, UT Austin and USACM superbly handled the duties of on-site secretariat. Susan Guthrie Lowrance of Helms Briscoe was instrumental in arranging for the conference venue, the Omni San Diego Hotel, and the social events. Cristina, Ruth and Susan were great resource to the conference co-chairs in many other matters. Partial sponsorship from Elsevier, Wiley, World Scientific, Springer, IACM, and USACM helped raise the quality of the social program. Of course, San Diego weather did not disappoint either: five days of sunshine and comfortable temperatures were a perfect complement to the already warm and friendly atmosphere of ACM 2013.

![](_page_32_Picture_9.jpeg)

*Figure 6: Tom Hughes during his closing remarks at the conference banquet*

In the closing remarks at the conference banquet the guest of honor, in turn, expressed his gratitude to everyone by saying, "This was one of the most memorable events in my  $l$ life."

![](_page_33_Picture_0.jpeg)

*for all inclusions under AMCA please contact: Victorio Sonzogni sonzogni@intec.unl.edu.ar http://amcaonline.org.ar*

#### *Argentine Association for Computational Mechanics*

**ENIEF 2013 ENIEF 2013 XX Congress on Numerical Methods and their Applications Mendoza, Argentina 18 - 22 November 2013**

The Argentine Association for Computational Mechanics (AMCA) announces the XX Congress on Numerical Methods and their Applications, which will be held in Mendoza, Argentina, organized by the National Technological University of Mendoza.

The Conference topics includes application of numerical methods in engineering problems, among which:

Fluid Mechanics, Solid Mechanics, Constitutive Modelling of Materials,Stability and Non Linear Structures, Structural Dynamics, Aerospatial Technology, Heat and Mass Transfer, Failure Modelling of Materials, Computational Geometry, Control and Optimization,Problems in Multiphysics, Simulation of Turbulent Flows, Teaching Numerical Methods in Engineering, Inverse Problems and Application, Industrial Applications, Wind Engineering, Multibody Systems, High Performance Computating in Computational Mechanics, Acoustics and Mechanical Vibrations, Uncertainties

![](_page_33_Picture_7.jpeg)

and Stochastic Modelling, Computational Modelling in Bioingeniería y Biomedical Systems, Numerical Simulation of Environmental Problems, Multiscale Modelling of Materials, Computer Methods in Seismic Engineering, Multiphase Flows, Structural Analysis.

#### *The relevant dates are:*

- Deadline for presenting a one-page abstract: *May 20, 2013*
- Acceptance of the one-page abstract: *June 3, 2013*
- Deadline for submitting the full length paper : *July 31, 2013*
- Acceptance of the full length paper: *August 31, 2013*
- Deadline for early payment: *September 15, 2013*
- Congress: *November 18-22, 2013*

*Figure 1: Mendoza City and the the Andes Mountain behind*

Mendoza is a beautiful city, in the mid-western Argentina, land of high mountains and fine wines. Mendoza holds the largest wine producing area in Latin America. As such, Mendoza is one of nine cities worldwide in the network of Great Capitals of Wine, and the city is an emerging enotourism (Wine tourism) destination and base for exploring the region's hundreds of wineries located along the Argentina Wine Route. Aconcagua Mount is the highest peak of America. From its 6,962

> m.a.s.l., it leads this entire province, where geography is generous in mountains, eternal snow, valleys, rivers, hotsprings, plains, deserts and magical oasis offering different tourist possibilities.

*More informations may be found at: Email:* enief2013@frm.utn.edu.ar Web: www.enief2013.frm.utn.edu.ar  $\bullet$ 

*Figure 2: Puente del Inca (Inca's bridge): natural formation at the Andes Mountain*

![](_page_33_Picture_21.jpeg)

### **New Research Centre in Computational Mechanics**

On March 14th 2013 a new independent Research Unit has been created in Argentina. The Research Centre in Computational Methods, CIMEC (for Centro de Investigación de Métodos Computacionales), has been created by agreement between the Argentinean National Council for Scientific and Technological Research (CONICET) and the National University of Littoral, Santa Fe, Argentina (UNL).

This unit has been created based on the former International Centre for Computational Methods in Engineering, which depended from the Institute for Technological Development of the Chemical Industry (INTEC). This is the first independent Research Unit from CONICET entirely dedicated to Computational Mechanics, and constitutes the largest research Institution in Argentina working in this field.

CIMEC has currently five research areas:

- Numerical Methods in Fluid Mechanics
- Numerical Methods in Fluid Structure Coupling
- Numerical Methods in Solids and Mechanisms
- **Bioengineering**
- Computer Methods and Programming Techniques

A total of fifty people are currently working in this new research unit, twenty of whom are researchers from CONICET or UNL. The group started working in 1980 within INTEC, and was founded by Prof Sergio Idelsohn. This group has gain reputation for its three decades of constant activity in the field, with publications in the most renowned scientific journals.

The Centre occupies a 500 sq meters modern building with a nice view over the Parana River, with spaces for its computers clusters and a conference room. This building will now be expanded to reach a total of 1250 sq meters thanks to a grant recently obtained from the Argentinean National Ministry of Science and Technology.

Researchers from CIMEC give support to the Postgraduate Program in Computational Mechanics of the UNL. The group has also gained strong recognition in Argentina for its activity in computational mechanics applications for industries all along the country, within which we can mention YPF, Yaciretá Binational Entity, Ternium-Siderar, Mahle Argentina SA, Nuclear Regulatory Authority, and many others.

This new era will give CIMEC a strong impulse to increase its productivity, develop stronger links with industry and produce new and exciting research in the field of Computational Mechanics

*Alberto Cardona Interim Director CIMEC*

> *Figure 3: Architects view of projected CIMEC building*

![](_page_34_Picture_15.jpeg)

*Figure 3: CIMEC building*

![](_page_34_Picture_17.jpeg)

![](_page_35_Picture_0.jpeg)

## bv:

*Pablo M. Jacovkis* Universidad Nacional de Tres de Febrero pjacovkis@untref.edu.ar  $and$ Universidad de Buenos Aires jacovkis@dc.uba.ar

## Sergio Idelsohn and the Development of **Computational Mechanics in Argentina**

Sergio is a world known specialist in numerical simulation of problems related to mechanical engineering, in particular in computational fluid dynamics, and is one of the developers of the Particle Finite Element Method (PFEM). His positions, prizes and grants include professorships at the National University of Rosario, the National University of the Littoral in Santa Fe, the Polytechnical University of Catalonia in Barcelona, the Institute of Advanced Study in Princeton, the University Paris VI Pierre et Marie Curie, the direction of the International Center for Numerical Methods in Engineering in Santa Fe, the Houssay Prize, the Konex Prize, the Scopus Prize, the SEMNI Prize, and a 2.5 million euro grant from the European Research Council.

Sergio graduated in 1970 at the National University of Rosario. That was a particularly complicated year in the ever complicated history of Argentina. The military dictatorship which ruled the country after having infamously overthrown the legal President Illia in 1966 (and having replaced the legal authorities of the Universities with people more interested in detecting communists and guerrillas than in improving teaching and science) began to be immersed in a process of instability. The first dictator, General Onganía, was himself overthrown in 1970 by General Levingston, who was in turn overthrown by General Lanusse in 1971. Curiously, some decisions of the dictatorship were positive: the University of Rosario, formerly part of the National University of the Littoral, had just been created as part of a policy of creating Universities in the country which permitted many young people to enroll as undergraduate students.

After graduating, Sergio wanted a scientific career. It was very unusual for engineers in Argentina to obtain a Ph. D., as most engineers thought of themselves as professionals, not scientists. So Sergio applied for several scholarships and accepted one in Liege, Belgium. (His former professor, Orengo, had heard about a new method, something called "the finite element method" and had bought a book on this subject, the first Zienkiewicz.)

It was not easy to study under the distinguished scholar Veubeke. He suggested a problem which, after one year, Sergio realized had no solution. When Sergio dared to tell him, he said "Yes, I agree, better work in this other problem". Despite this, he succeeded in finishing his Ph. D. dissertation in three years, and in 1974 returned to Argentina.

Those were difficult years in Argentina, politically, economically and personally. He had a part-time position at the School of Engineering of the University of Rosario (thanks to Orengo). He taught at the Faculty of Economics and, by night, at the Technological University. After the 1973 election, the military had (provisionally) retired from government, the formerly ousted President General Perón was President again, and a paramilitary group, the "three A" (Argentine Anticommunist Alliance), began murdering political opponents and supposed friends of the guerrilla. Perón died in July 1974 and was replaced by his wife, Isabel Martínez de Perón. Living in Argentina and belonging to the University became very uncomfortable. People were afraid, and the situation worsened. In 1976 the military, with the desire of exterminating the guerrilla, overthrew the government, and the bloodiest dictatorship in contemporary Argentina (General Videla's) started. Sergio´s economic situation worsened

Figure 1: **First ENIEF in** Bariloche, Argentina, July1983, with the participation of **Professor Richard** Gallagher

![](_page_35_Picture_11.jpeg)

and eventually, after five extremely difficult years, Sergio accepted a postdoctoral scholarship from the CONICET (National Council for Scientific and Technical Research), and in 1979 they returned to Liege where he knew people who could help him get an academic position.

In 1980, things began to improve. The worst period was over, although killings and disappearance of people continued until a civilian President, Raúl Alfonsín was elected. Alberto Cassano offered him a position in Santa Fe to organize a scientific group in mechanics in the Institute for Technological Development in Chemical Industries (INTEC), founded by Dr Cassano. So in 1981 Sergio and his family where re-installed in Santa Fe, working at INTEC. Here Sergio's scientific career in Argentina truly began. In 1983 the Bariloche group (whose director was Sergio Pissanetzky) organized a course on finite elements jointly with ENIEF'83, the first National Meeting of Researchers and Users of the Finite Element Method, and Sergio was invited to this meeting, as was the late professor Richard Gallagher. Both Sergios decided to organize ENIEF on a regular basis. New ENIEFs took place in Bariloche in 1984 and 1985.

Meanwhile, in 1981 profess. Gallagher, Oden and Zienkiewicz established the IACM. The idea naturally appeared to Idelsohn and other scientists to establish a similar society in Argentina, which would be a member of IACM. In 1985 the AMCA was created; Sergio was its first President and remained so for 20 years. Sergio was simultaneously becoming an outstanding and internationally prestigious scientist, thanks not only to his brilliant personal career but also to his successful efforts in creating an important center of research in Santa Fe, where many distinguished scientists and disciples of Sergio's worked.

In December 1983 the political difficulties ceased in Argentina, when the new democratic Alfonsín administration was inaugurated. But nothing was simple compared to research in other countries. On the one hand,

during the first years of democracy, it was uncertain whether the government would be overthrown by a new coup d'état, and many scientists and intellectuals did not know whether they would need to go abroad again. On the other hand, the scientific budget was still scarce, and for many scientists going abroad, this time for economic, not political, reasons, was the only option. Sergio remained in Santa Fe, sometimes maintaining intermittent visiting positions abroad, and with his usual optimism managed to transform the small community of CM specialists into an important group, aiding not only Santa Fe but also other regions. (He was also a consultant for several national or provincial agencies and private firms.)

In 1986, the 4th ENIEF took place in Bariloche, organized by Luis Godoy from Córdoba. Luis invited the Spanish scientist Eugenio Oñate to Bariloche. Sergio and Eugenio met and began a productive scientific collaboration that continues hitherto; the "Barcelona-Santa Fe" axis has become a rich bi-national scientific joint venture of which both countries may be proud.

But Argentina is a very curious country. Just when, in the last decade, the government began to significantly back science, both financially and politically, some bureaucratic authority at the CONICET decided that Sergio should not be allowed to spend part of the year in Barcelona. Needless to say, many scientists in many countries spend part of the year abroad, with no objections but often encouragement. So in 2006 Sergio was fired from CONICET (but not from the University of the Littoral). However, Sergio continues collaborating with Santa Fe and Argentina.

Sergio Idelsohn's scientific merits are internationally known. What is perhaps less known, both in and out of Argentina, in circles of younger researchers who (fortunately) did not live through the dark years of military dictatorships and instability, and then through the years with minimum budgetary support, is that being successful in Argentina, both as a teacher, a scientist, a scientific manager and a specialist in preparing human resources, requires fighting against all odds, and a will and a strength that few people have, and which Sergio has.

Figure 2: Fisrt meeting of Eugenio Oñate with Sergio Idelsohn in

![](_page_36_Picture_9.jpeg)

Figure 3: Prof. Olek Zienkiewicz visiting Santa Fe (center) with Victorio Sonzogni and Sergio Idelsohn, Argentina, February 1987

![](_page_36_Picture_11.jpeg)

![](_page_37_Picture_0.jpeg)

*for all inclusions under abmec please contact: Gray Farias Moita gray@dppg.cefetmg.br*

![](_page_37_Picture_2.jpeg)

NOVEMBER 10-13, 2013. PIRENÓPOLIS-GO

**XXXIV CILAMCE**<br>The Ibero Latin American Congress on Computational Methods in Engineering The Ibero Latin American Congress on Computational Methods in Engineering<br>
(CILAMCE) is a series of annual meetings on computational methods in engineering, promoted by the Brazilian Association of Computational Methods in Engineering (ABMEC), intended to provide an international opportunity for communicating recent developments in various areas of numerical methods. Since 1977 the CILAMCE provides a forum for engineers, students, researchers and other professionals active in the field of numerical methods, coming from Brazil and other countries, to discuss and to explore the state-of-the-art of recent applications of computational methods in several engineering branches. The framework of CILAMCE is multidisciplinary and scientists from all over the world are encouraged to contribute in the conference. The technical program includes plenary speakers and mini-symposia sessions on pre-defined topics with contributing papers on this scientific field.

After 33 successful meetings, the 34th Ibero-Latin American Congress on Computational Methods in Engineering will be held in November 10-13, 2013 at Pousada dos Pirineus Resort, located in the charming city of Pirenópolis, and hosted by the Graduate program in Geotechnics, Structures and Civil Construction (PPG-GECON) of the Federal University of Goiás (UFG). Pirenópolis is located in the state of Goiás, Brazil, and about 150 km far from Brasilia and about 120 km far from Goiânia. Its unique ambiance, nature and typical cuisine have made the city a favorite travel destination.

On behalf of the organizing committee of CILAMCE 2013, it is a great pleasure to invite you to the XXXIV Ibero-Latin American Congress on Computational Methods in Engineering. We look forward to welcoming you to Pirenópolis at CILAMCE 2013. ●

#### **Leopoldo Luis Cabo Penna Franca (April 7th, 1959 - September 19th, 2012)**

Leopoldo (Leo) Franca graduated in Mechanical Engineering at the Pontifical Catholic University of Rio de Janeiro in 1981, obtained his M.Sc. in Mechanical Engineering at the Pontifical Catholic University of Rio de Janeiro in 1983 and his Ph.D. in Mechanical Engineering at Stanford University in 1987 under the supervision of Prof. T.J.R. Hughes. His experience in Mechanical Engineering with emphasis in Numerical Methods, allowed him to act, among others, on the following subjects: stabilized methods for fluids, solids and acoustics, residual-free methods and methods for enhanced transport equations. Leo's publication record includes works on stabilized methods, Galerkin least squares methods, unusual stabilized methods, residual-free bubbles, discontinuous enrichment methods and Petrov–Galerkin enrichment methods. He published over 100 papers in journals and conference proceedings. His body of work has received over 3,900 citations according to the ISI Web of Knowledge and he is listed as an ISI Highly Cited Author. Leo Franca received the R.H. Gallagher Young Investigator award sponsored by the US Association for Computational Mechanics (1999). He was also elected Fellow by the International Association for Computational Mechanics, IACM (2002) and Fellow by the USACM (2007). Leo was an active member of the Advisory Board of IJNME and CMAME.

His brilliant career started with a research position at the National Laboratory for Scientific Computation (LNCC) in Brazil from 1988 until 1993 when he moved abroad, taking a Visiting Professor position at Purdue University (1993) and later at the University of Colorado at Denver (CU-Denver) from 1994 to 2009. There, at the Colorado University, he started as an Associate Professor, becoming Director of the Center for Computational Mathematics (1996–1999), and promoted to full Professor in 1999. While at CU-Denver, Leo struggled against a severe liver disease, caused by Wilson's disease, which required a liver transplant he could finally accomplish in 2004, at the University of Colorado Hospital. About this, he wrote on his Facebook wall: ''It was a dramatic year. I spent one year waiting for a liver transplant. Towards the end I was having a series of liver failures until I completely passed out. The doctor told my wife I had 3 days to live, and he was hoping a liver would appear. It did! And all ended well!''.

Back to Brazil, he joined the Civil Engineering Department of the Alberto Luiz Coimbra Institute for Graduate Studies and Research (COPPE) at the Federal University of Rio de Janeiro (UFRJ) as Visiting Professor, from 2008 to 2010 where, during this term, he joined our team at the High Performance Computing Center at COPPE/UFRJ, collaborating as a consultant in R&D projects for the oil industry. Many fruitful meetings and discussions with Leo around themes such as fluid-structure interaction and its underlying intricacies provided deeper insight into the problem and, by all means, enjoyable moments to be remembered by all team members.

![](_page_37_Picture_12.jpeg)

For a brief period, in 2011, he returned to LNCC as a Visiting Professor. Late in 2011, he joined the new IBM Research Lab in Brazil, the first IBM Research Lab in the Southern Hemisphere, where he joined its Smarter Natural Resources Discovery department as Senior Research Scientist, participating in several worldwide R&D projects in Computational Mechanics applied to the oil industry. He will be missed a great deal by the so many friends, colleagues and students he captivated throughout his very active live. We extend our sympathies to Lucia, his wife, to Louise and Lais, their daughters, and to all his family. It was a great privilege to have known him.

*José Luis Drummond Alves, Alvaro L.G.A. Coutinho and Fernando A. Rochinha*

## **WCCM in São Paulo <u>– an event with Brazilian flavor-</u>**

The X WCCM (10th World Congress on Computational Mechanics),<br>jointly with the XXXIII CILAMCE (33rd Iberian Latin-American Congress on Computational Methods in Engineering), was held in the vibrant city of São Paulo, Brazil during July 8-13, 2012 under the auspices of the Brazilian Association for Computational Methods in Engineering (ABMEC) and the International Association for Computational Mechanics (IACM).

Despite international and national difficulties, the organizing agency SOMA, the local organizing committee and the scientific committees achieved an outstanding, enjoyable and memorable congress. With 9 plenary and 30 semi-plenary lectures by distinctive colleagues and over 1800 presentations organized within 178 mini-symposia and gathered into 14 technical sessions distributed in 26 rooms, the WCCM 2012 was the biggest scientific Engineering congress ever made in Brazil. With participants from 92 different countries, Brazil topped the list with 550 delegates, followed by USA with 360, Japan with 120, Germany and France with 90 each.

The congress took place at the Hotel Transamerica in São Paulo, Brazil. The cosmopolitan São Paulo, the 4th largest city in the world with more than 20 million inhabitants, covering an area of nearly 1,500 km2, has offered a plentiful choice of entertainment to the participants.

The Opening Ceremony took place at Sala São Paulo, the city´s most prestigious concert hall. It is allocated in the former Sorocabana Train Station, built in 1926 for the transportation of coffee to the harbor of Santos. For an audience of 900 hundred people, the Chamber Orchestra of the University of São Paulo, conducted by Gil Jardim, offered a Brazilian music concert with the world famous Italian chromatic harmonica soloist Gianluca Littera.

The congress was sponsored by the Polytechnic School at University of São Paulo, the state agency FAPESP and the federal agencies CNPq and CAPES, and companies like Petrobrás, ANSYS, ESSS, Embraer and Engevix. The USACM supported the congress through the provision of 50 travel grants for North-American students and young investigators. The ABMEC also supported through the concession of 350 scholarships to Latin-American students and young investigators.

The Festa Brasileira on Thursday night was the high point of the social program. After a banquet for 1200 participants with exclusively Brazilian drinks and food, a show with the Bossa Nova star Toquinho was presented. The night was closed by a Carnival parade of the Escola de Samba Rosas de Ouro. Many of our colleagues danced samba until late in the night!  $\bullet$ 

> *by P.M. Pimenta,Conference Chairman ppimenta@usp.br*

![](_page_38_Picture_8.jpeg)

*Figure 6: Mr & Mrs Coutinho, Mr & Mrs Liu,* 

![](_page_38_Picture_10.jpeg)

![](_page_38_Picture_11.jpeg)

#### *Figure 1:*

*Opening Ceremony, from left to right: Prof José Roberto Cardoso (Dean of the Polytechnic School), Prof Genki Yagawa (President of IACM), Mr Gilberto Kassab (Mayor of São Paulo), Prof José Luis Alves (President of ABMEC) and Prof Paulo Pimenta*

![](_page_38_Picture_14.jpeg)

*Figure 2: Audience at Opening Ceremony*

![](_page_38_Picture_16.jpeg)

*Figure 3: Chamber Orchestra of University of São Paulo, Gil Jardim (conductor) & Gianluca Littera (soloist)*

![](_page_38_Picture_18.jpeg)

*Figure 4: Plenary lecture by Prof Hughes*

![](_page_38_Picture_20.jpeg)

*Figure 5: From left to right: Prof Wriggers, Prof Pimenta, samba girl & Prof Campello*

*Bossa Nova show by Toquinho*

![](_page_39_Picture_0.jpeg)

erman Associaton for Computational Mechanics

![](_page_39_Picture_2.jpeg)

*for all inclusions under* **GACM** *please contact:*

**Wolfgang A. Wall** wall@lnm.mw.tum.de

![](_page_39_Picture_5.jpeg)

#### **Ekkehard Ramm elected as Honorary Chairman of GACM**

**During the last member assembly of the German Association of Computational**<br>Mechanics at the ECCOMAS Congress in Vienna in September 2012, Professor Ekkehard Ramm has been elected as Honorary Chairman of the Association. This very rare and special distinction has been unanonymously supported by the members of GACM and recognizes his dedicated and long time work for GACM.

Ekkehard Ramm was a GACM member from the very start of the Association and over the years has permanently served not only GACM but also the broader community in Computational Mechanics. He became President of GACM in 2000 and his two term service as President until 2008 marked a very fruitful time for GACM. Not only the number of full members grew substantially but also a number of new initiatives have been taken that are still in place today and by this form a kind of heritage of his presidency. Two examples are the start of the GACM Report, and the beginning of a very successful and timely conference series - the GACM Colloquia for Young Scientists from Academia and Industry. These conferences and their success became the inspiration for a similar series on the European level, the ECCOMAS Young Investor Conference (YIC). Ekkehard Ramm also was very active on the European (within ECCOMAS) and the international level (IACM) where he not only represented GACM interests. He not at all served his personal interests but always had a broader, holistic point of view; he always works for a sustained development of the community. The GACM Executive Council is happy to enjoy his advise also in the future.

*The new GACM Honorary Chairman Ekkehard Ramm felicitated by Peter Wriggers and Wolfgang A. Wall (past and present Presidents of GACM)*

### **New GACM Executive Council took office in January 2013**

At the general meeting of GACM, that took place in September 2012, a new Executive Council has been elected unanonymously. The new team took office in January 2013 for a four year term according to the GACM bylaws. **Wolfgang A. Wall** from TU München, vice president of GACM in the last four years, has been elected as the new president and **Michael Kaliske** from TU Dresden has been elected as the new vice president.

Further members of the EC are: **Marek Behr** from RWTH Aachen (representing CFD and CSE), **Sven Klinkel** from RWTH Aachen (Treasurer), **Sigrid Leyendecker** from FAU Erlangen-Nürnberg (representing Mathematics and Dynamics), **Thomas Münz** from DynaMore (representing industry) and **Peter Wriggers** from LU Hannover (as past president). **Lena Yoshihara** from TU München will act as the new Secretary General and during her maternity leave she will be substituted by **Alexander Popp** from TU München.  $\bullet$ 

![](_page_39_Picture_13.jpeg)

![](_page_39_Picture_14.jpeg)

*Wolfgang A. Wall*

*Michael Kaliske*

![](_page_39_Picture_17.jpeg)

![](_page_39_Picture_18.jpeg)

![](_page_39_Picture_19.jpeg)

![](_page_39_Picture_20.jpeg)

![](_page_39_Picture_21.jpeg)

![](_page_39_Picture_22.jpeg)

![](_page_39_Picture_23.jpeg)

![](_page_39_Picture_24.jpeg)

*Alexander Popp*

*Marek Behr*

*Sven Klinkel*

*Sigrid Leyendecker* *Thomas Münz*

*Peter Wriggers*

## **Prestigious European Awards go to GACM Members Prestigious European Awards go to GACM Members**

2012 marked a very successful year for GACM as the following two impressive examples demonstrate.

Prof. em. Dr.-Ing. habil. Dr.-Ing. E.h. Dr. h.c. mult. **Erwin Stein**, from the Leibniz University Hannover, received the highest award given by ECCOMAS, namely the Ritz-Galerkin medal. The award ceremony took place at the opening of the ECCOMAS congress in September 2012 in the main concert hall of the Vienna Musikverein.

Another reason for celebration for GACM was the fact that the ECCOMAS

![](_page_40_Picture_4.jpeg)

*Erwin Stein Lena Yoshihara*

![](_page_40_Picture_6.jpeg)

PhD award for the best PhD thesis in the field of Computational Methods in Applied Sciences and Engineering went to an awardee from Germany for the first time.

![](_page_40_Picture_9.jpeg)

Dr.-Ing **Lena Wiechert** (now Yoshihara) from Technische Universität München received this award for her thesis entitled "Computational modeling of multi-field and multi-scale phenomena in respiratory mechanics".  $\bullet$ 

### *GACM holds the next Colloquium on Computational Mechanics in Hamburg*

The fifths edition of the successful series of GACM Colloquia on Computational Mechanics for Young Scientists from Academia and Industry will be held at the Campus of the Hamburg University of Technology from **September 30 to October 2, 2013**. The Chairmen of this years Colloquium (A. Düster, E. Kreuzer, O. von Estorff, N. Hoffmann, S. Bargmann from TUHH) together with the local organizing committee (M.-A. Pick, S. Brändli, M. Abele, P. Erbts) are well on their way for another successful meeting and have put together a promising program.

According to the tradition of this meeting two keynote lectures are given from outstanding senior researchers from academia, one from abroad and one from Germany, and one keynote lecture from a representative from industry. This year partcipants will enjoy a keynote lecture by Robert L. Taylor from UC Berkely, one from Karl Schweizerhof from Karlsruhe Insitute of Technology and one from Christian Cabos from Germanischer Lloyd.

In addition the program will feature among others 17 minisymposia on a broad range of interesting topics organized by young scientists for young scientists. Highlight of the social program are a harbor cruise and the conference dinner on board of a decommissioned light vessel.

![](_page_40_Picture_15.jpeg)

More details on the colloquium can be found at http://www.tuhh.de/gacm2013/.  $\bullet$ 

#### *The Aachen Conference on Computational Engineering Science*

The Aachen Conference on Computational Engineering Science (AC.CES) will be held on **September 9-11, 2013** at the RWTH Aachen University and will bring together leading experts in theory, method development, and applications related to problems in computational engineering. The main objectives of the conference are to present cutting-edge research and to facilitate interdisciplinary collaboration. The conference consists of a series of plenary sessions featuring invited talks by leading experts. The plenary sessions will be accompanied by poster presentations of regular participants.

Conference topics are: uncertainty quantification, inverse problems in materials science, computational biology, model order reduction, optimization and control and imaging/tomographic inversion.

![](_page_40_Picture_20.jpeg)

![](_page_40_Picture_21.jpeg)

For more information please visit: **www.ac-ces.rwth-aachen.de**  or contact the conference secretariat at **acces@aices.rwth-aachen.de. ●** 

![](_page_41_Picture_0.jpeg)

*for all inclusions under KSCM pleace contact: Moon-Ki Kim* mkkim1212@skku.edu

## **Korean Society for Computational Mechanics**

The first workshop of **Korean Society for Computational Mechanics (KSCM)**<br>was recently held on February 25-26, 2013, in YongPyong Ski Resort, which is the most beautiful ski area in Korea and also the official site of PyeongChang 2018 Winter Olympic Games.

Eight distinguished invited speakers presented special topics covering from nanomechanics to aerodynamics simulation and large-scale parallel computation

**APACM** 

before more than 100 members. In addition, a special tutorial session on multi-scale framework for lithium-ion battery design followed.

Professor Sung-Kie Youn, President of KSCM, reported the hosting process of 2016 World Congress on Computational Mechanics (WCCM2016) and began to organize the Local Committee of WCCM2016. He also discussed the future prospects of the society.

As the host organization of the 6th Asia Pacific Congress on Computational Mechanics (APCOM2016), which will be jointly held with WCCM2016, KSCM recently launched the official

*Figure 1: The official website of the Asian Pacific Association for Computational Mechanics (http://apacm-association.org)*

website of the Asian Pacific Association for Computational Mechanics (APACM) at **http://apacm-association.org**. It is expected that all participating organizations in APACM not only share the news much easier, but also establish concrete friendships with each other through this site. Also, KSCM opened its own website at **http://kscm-society.org**. Until the official website of WCCM2016 is opened

![](_page_41_Picture_11.jpeg)

right after WCCM2013, this website will be a hub of domestic communication among KSCM members and WCCM2016 Local Organization Committee.

KSCM fixed the dates and venue for **WCCM2016**. It will be held in COEX complex, a business and cultural hub located in the heart of *"Gangnam style"*, on **July 24~29, 2016**. This massive complex consists of 12 buildings including World Trade Center Seoul, City Airport Terminal, three luxury hotels, musical theater, COEX aquarium, Asia's largest underground shopping center, and COEX convention center hosting 200 exhibition and 2,000 conferences every year including G20 Seoul Summit and 2002 FIFA World Cup. ●

*Figure 2: The official website of KSCM (http://kscm-society.org)*

![](_page_41_Picture_15.jpeg)

*Figure 3: COEX complex, the venue of WCCM2016*

![](_page_41_Picture_17.jpeg)

*Figure 4: Participants to the first KSCM Computational Mechanics Workshop at YongPyong Ski Resort, Korea*

## conference diary planner

![](_page_42_Picture_343.jpeg)

![](_page_43_Picture_0.jpeg)

**IACM and ECCOMAS** are pleased to announce the joint organization of

![](_page_43_Picture_2.jpeg)

11th. World Congress on **Computational Mechanics** (WCCM XI)

and

5th. European Conference on **Computational Mechanics<br>(ECCM V)** 

**6th. European Conference on Computational Fluid Dynamics** (ECFD VI)

![](_page_43_Picture_7.jpeg)

20 - 25 July 2014 - Barcelona, Spain www.wccm-eccm-ecfd2014.org