

## expressions

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Structural Analysis with the Finite Element Method Linear Statics, Volume 2: Beams, Plates & Shells Book Review by D. Givoli

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The word "computational" is increasingly used to identify branches of classical science and technology fields that focus on quantification aspects with the help of numerical methods and modern computers. The name Computational Mechanics was coined in 1985 (30 years ago!) and probably was the first of a series of similar initiatives in a many fields that merged their original name with the word "computational" (i.e. physics, chemistry, biology, biomechanics, materials science, geosciences, linguistics, neurosciences, etc.). In the latest issue of IACM Expressions we presented the "computational thinking" initiative as an attempt to integrating computational ideas and attitudes into other disciplines and in education.

One of the recent incorporations to the broad computational community is the so-called "computational pathology" action. This has been defined as "an approach to medical diagnosis that incorporates multiple sources of raw data (eg. clinical electronic, medical records, laboratory data, including "-omics", and imaging); extracts biologically and clinically relevant information from those data; uses mathematical models at the levels of molecules, individuals, and populations to generate diagnostic inferences and predictions, and presents that clinically actionable knowledge to customers through dynamic and integrated reports and interfaces, enabling physicians, patients, laboratory personnel, and other health care system stakeholders to make the best possible medical decisions" (D.N. Louis et al., Computational Pathology. An emerging definition. Arch Pathol Lab Med, Vol. 138, 1133-1138, September 2014).

Surely we will hear more about this new member of the "computational family" that indeed shares many disciplines and interests with other existing members of the family, and, in particular, with the computational biomechanics field. On a different topic, one of the most remarkable events supported by the IACM in 2015 has been the 1st Pan American Conference on Computational Mechanics (PANACM). PANACM 2015 was held on April 27-29 in Buenos Aires (Argentina) aiming to bring together the large community of members in computational mechanics in the Americas.

The PANACM conference was very successful and attracted some 600 participants from 38 countries, including some 100 participants from Europe and 30 from the Asia-Pacific region. The conference aims to fill the American gap of the so-called regional conferences of the IACM, such as the ECCOMAS and APCOM conferences held respectively in Europe and the Asia-Pacific region at every four year intervals. You can read more about PANACM 2015 in the pages of this bulletin.

2015 was another year full of scientific events of interest to the computational mechanics community. As an example 31 thematic conferences on different computational topics were held in several European countries and in the US. This was in addition to some 15 national conferences organized by the IACM affiliated organizations all over the world. All together this is a good sign of the vitality of the field and of the IACM.

The next big IACM event will be the XII World Congress on Computational Mechanics to be held in Seoul (Korea) on 24-29 July 2016. The congress will run simultaneously with the 6th Asian Pacific Congress on Computational Mechanics. This promises to be another interesting event that will gather the computational community from the five continents. I encourage you to participate in WCCM2016 in Seoul. Editor of IACM Expressions

# Brownian Dynamics Simulation of Cellular Protein Networks

by <u>Kei W. Müller,</u> <u>Christoph Meier,</u> and Wolfgang A. Wall

" ... we have succeeded in unearthing fundamental mechanisms, which enable the cell to create tailormade network architectures with unique mechanical properties in order to react quickly and flexibly within its dynamic and ever-changing habítat.

ells are the base unit of life and Cbelong to one of three kingdoms: bacteria, archaea, and eukaryotes [1]. Among them, eukaryotic cells are the most complex as they alone can exist as highly specialized building blocks of multi-celled organisms, e.g., a human being. Despite a vast variety in form and function, a eukaryotic cell's structural blueprint is generic. One of its most important components is the cytoskeleton, a complex cross-linked biopolymer network, which is suspended in an aqueous medium, the cytoplasm, and consists of different species of slender protein filaments, e.g., semiflexible actin filaments (f-actin) and cross-linking molecules (linkers). It provides for a multitude of crucial cellular functions and, as a consequence, has received considerable scientific appreciation over the past decades. Besides enabling the adhesion and crawling of cells as well as the orchestration of cell division and migration, the cytoskeleton catalyzes metabolic activities and serves as the cell's sensory organ.

Despite mutual endeavors of various scientific disciplines, the mechanics of the cytoskeleton remain poorly explored in many aspects. Overcoming increasingly complex problems requires the joint efforts of experimentalists, theorists, and numerical engineers. Recently, mesoscale simulations of cross-linked networks made of mechanically coarsegrained filaments have emerged as a powerful instrument to interpret experiments and to validate physical theories. They enable the discovery of mechanisms behind the cell's ability to elegantly manipulate the structure of its cytoskeleton and to precisely tune its mechanical properties.

The simulation of cross-linked semiflexible networks has to meet three fundamental requirements. The mechanical description of highly slender filaments demands a mathematically rigorous theoretical model. Second, the computational performance must enable the modeling of large systems (hundreds of filaments and thousands of linkers in a volume of  $10^2$ - $10^3\mu$ m<sup>3</sup>) over a biologically relevant period of time ( $\geq 100$ s). Lastly, it is absolutely paramount to capture both the effect of thermal noise and viscous drag on filaments and linkers as they govern the mechanics on this length scale.

So far, a comprehensive solution for a Brownian dynamics (BD) approach meeting all requirements has not been presented. Besides a general lack of computational efficiency, current solutions mostly either do not capture parts of the relevant physics and/or have a heuristic rather than a strong theoretical foundation such as the many variations of wormlike chain approximations, e.g., bead-spring and bead-rod models (e.g., [2-5]).

Concerning the mechanical modeling of filaments and linkers, we apply the theory of one-dimensional continua, so-called Cosserat continua. On the one hand, this theory is capable of describing all relevant mechanical effects with sufficient accuracy. On the other hand, it allows for very efficient numerical solution procedures. In our case, we apply the Finite Element Method based on so-called geometrically exact beam elements [6, 7] and an implicit time integration scheme in order to solve the mathematical problem stemming from this continuum model.

However, it is not sufficient to solely model the filaments and linkers as individual instruments since we are interested in their interplay within the cytoskeletal orchestra. Concretely, this means that we also have to model the chemical bonds between filaments and linkers as well as the exchange of energy and momentum due to filament-filament collisions (so-called steric or contact interactions). Even though the practical interpretation of steric interaction is as simple as forbidding bodies to penetrate each other, its accurate, efficient, and robust numerical realization is far from trivial. In our simulations, we integrate chemical bonds as equality constraints and steric interactions as inequality constraints

consistently embedded into a mathematically sound variational framework. Considering the numerical effort resulting from the large time scales and system sizes, which are required to make physically relevant statements, numerical efficiency is most crucial in order to enable such simulations in a practically feasible manner. This is a distinctive advantage as compared to alternative methods that can be found in the literature (e.g., [4, 5]). We meticulously verified the theoretical and mechanical consistency of our approach, e.g., by validating the contact algorithm in highly demanding scenarios (Fig. 1), which bear significant relevance far beyond biophysical applications, e.g., when modeling the mechanics of ropes, fabrics, or macroscopic fibrous composites.

Having at hand an efficient simulation framework based on accurate models of the mechanical base units (filaments and linkers) and their interaction, we finally ensure the third fundamental requirement mentioned above: the correct representation of the governing physics on the microscopic scale. Keeping the balance between the effects of spatially and temporally uncorrelated thermal excitations and viscous drag as shown in Fig. 2, we ensure the satisfaction of the so-called fluctuation-dissipation theorem on the filament scale [8]. This theorem proposes the energetic balance between spontaneous displacements of a particle (heat→kinetic energy) and dissipation by drag (kinetic energy  $\rightarrow$  heat).

 $f_{visc}$ 

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In a cellular environment, the thermal excitations originate from random molecular collisions between the small fluid molecules of the cytoplasm and suspended microstructures, e.g., filaments. We model these excitations by means of the stationary, independent increments of a multi-dimensional standard Wiener process. The consistent inclusion of stochasticity into a simulation framework with implicit time integration is non-trivial and requires special attention and consideration [8]. Employing an effective, anisotropic, velocity-dependent drag law captures the viscous drag a filament experiences while moving through the fluid.

Based upon this validated filament model [9, 10], we have enhanced BD simulations towards applications on the network scale [11] where linker dynamics and the reaction kinetics of filaments and linkers are accounted for in a physically and chemically consistent manner. Like the filaments, linkers are subject to stochastic and viscous forces. Linkers and filaments can establish chemical bonds, whose occurrence and dissociation depends on spatial, geometrical, and stochastic criteria: Given that the first two criteria are met, the reaction is governed by a Poisson process.

 $m{m}_{visc}$ 

 $m{m}_{stoch}$ 

#### Figures 1:

Hexagonal arrangement of seven thin fibers, which are discretized with geometrically exact beam elements. The top panel depicts the initial configuration. When twisting the fibers, they come into contact with one another, which results in the configuration shown in the bottom panel

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## Figures 2:

Coarse-grained mechanical continuum description of a filament and external forces of stochastic and viscous origin acting on it

 $f_{stoch}$ 



## Figure 3:

Equilibrium phase diagram of cross-linked semiflexible polymer networks (center). Depending on the linkerto-binding-site ratio ni~R, four distinct morphologies can be observed, which are shown left and right of the phase diagram

The approach easily handles filament concentrations up to an f-actin equivalent of  $8-12\mu$ M - values commonly encountered in vivo and in in vitro experiments (e.g., [12]). Simulations were carried out in periodic volumes the size of small cells ( $6^3-10^3\mu$ m<sup>3</sup>) over time intervals spanning several thousands of seconds [13, 14], in many cases excelling current state-of-the-art approaches by a hundred up to more than a thousand times in terms of computational efficiency.

Having set the board for complex biophysical applications, we first studied the so-called *polymorphism* of the actin cytoskeleton, i.e., its morphological variety. Based on few fundamental assumptions concerning the linker, we established the equilibrium phase diagram of self-assembled network morphologies [15] shown in the central panel of Fig. 3. It predicts the emergence of four archetypes: isotropic-homogeneous networks, networks of bundles, clusters, and lamellae. We claim that the entropic competition between filaments and linkers is the driving agent of network selfassembly. It is encouraging that all of the morphologies we found have been observed in vitro [16] or in vivo [17].

Starting with an ensemble of randomly oriented, initially straight filaments, we simulated the process of thermal equilibration of the filaments in the presence of various linker concentrations. Filaments and linkers are confined in a cubic volume with periodic boundary conditions, which ensures constant concentrations and facilitates the use of statistical measures, e.g., structural correlation functions.

Knowing the key parameters of network self-assembly, we created one of the most common and important network structures in cells, bundled networks, in order to study its rheology. Networks of bundles occur, e.g., in filopodia or stress fibers. Given a reasonable mechanical parameterization of the linker, we only need to set the correct ratio  $R=c_l/c_f$  of linker and filament concentrations to see the desired morphology develop. Typically, the first phase of in silico rheological studies is the simulation of network evolution. Well-developed networks emerge after ~1000-1500 simulated seconds. The result of this first phase is a bundle network such as the one depicted in *Fig. 4*.

The wide range of mechanical properties of the cytoskeleton stems from the transient nature of the linker-filament bond [16]. Therefore, we probed the networks' rheology across a broad frequency band and arrived at a comprehensive rheological spectrum for bundle networks spanning ten orders of magnitude in rescaled frequency space (unscaled: 0.003-105Hz) with previously unknown properties [13] (Fig. 5). We found three distinct frequency-dependent mechanical domains: a high-frequency regime where the viscoelastic moduli display a new, bundle-specific power law behavior, a strongly linker-specific intermediate-frequency, and a lowfrequency regime where we detected network rearrangements and the collective motion of the entire network structure. As Fig. 5 shows, our findings concerning the latter two regimes are in excellent agreement with experiments [18, 19]. We were able to confirm the general low-frequency scaling behavior of G',G"~ $\omega^{1/2}$ , and we are fully capable of modeling biologically most relevant biopolymer architectures such as actin-fascin networks.

Interestingly, the high-frequency regime is inaccessible by means of current experimental techniques. Here, our simulations support the theoretically well-founded claim that we have in fact discovered a previously unknown material behavior as we find a clear deviation from the commonly accepted G',G"~ $\omega^{3/4}$ behavior of the viscoelastic moduli (*Fig. 5*).

By means of highly efficient finite element simulations, we have succeeded in unearthing fundamental mechanisms, which enable the cell to create tailormade network architectures with unique mechanical properties in order to react quickly and flexibly within its dynamic and ever-changing habitat. Furthermore, we have made a case for the importance of innovative and well-engineered simulation techniques to the natural



## Figure 4:

A network of cross-linked bundles, which is confined in a periodic volume of edge length 6µm. The simulated time leading up to this network geometry is ~1500s

sciences. Our recent efforts, however, only represent the first steps into a vast field of challenging and innovative applications of our approach in biophysics and material science.



10<sup>1</sup>

 $10^{2}$ 

 $\omega/\omega^*$ 

 $10^{3}$ 

10<sup>4</sup>

## References

- Alberts, B., et al., Molecular biology of the cell, ed. M.G. Anderson, S. 2008: Garland Science. 1
- 2. Onck, P.R., et al., Alternative explanation of stiffening in cross-linked semiflexible networks. Phys Rev Lett, 2005. 95(17): p. 178102.
- 3. Zagar, G., P.R. Onck, and E. van der Giessen, Elasticity of rigidly cross-linked networks of athermal filaments. Macromolecules, 2011. 44: p. 7026-7033.
- 4 Kim, T., W. Hwang, and R.D. Kamm, Dynamic role of cross-linking proteins in actin rheology. Biophys J, 2011. 101(7): p. 1597-1603.
- Kim, T., et al., Computational analysis of viscoelastic properties of crosslinked actin networks. PLoS Comput Biol, 5 2009. 5(7): p. e1000439.
- Meier, C., A. Popp, and W.A. Wall, A locking-free finite element formulation and reduced models for geometrically exact 6. Kirchhoff rods. Comput Method Appl M, 2015. 290: p. 314-341.

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- 7. Meier, C., A. Popp, and W.A. Wall, An objective 3D large deformation finite element formulation for geometrically exact curved Kirchhoff rods. Comput Method Appl M, 2014. 278: p. 445-478.
- 8. Cyron, C.J. and W.A. Wall, Numerical method for the simulation of the Brownian dynamics of rod-like microstructures with three-dimensional nonlinear beam elements. Int J Numer Meth Eng, 2012. 90(8): p. 955-987.
- 9. Cyron, C.J. and W.A. Wall, Finite-element approach to Brownian dynamics of polymers. Phys Rev E Stat Nonlin Soft Matter Phys, 2009. 80(6): p. 066704.
- 10. Cyron, C.J. and W.A. Wall, Consistent finite-element approach to Brownian polymer dynamics with anisotropic friction. Phys Rev E Stat Nonlin Soft Matter Phys, 2010. 82(6): p. 066705.
- Cyron, C.J., et al., Micromechanical simulations of biopolymer networks with finite elements. 11.
- J Comput Phys, 2013. 244: p. 236-251.
- 12. Lieleg, O., et al., Transient binding and dissipation in cross-linked actin networks. Phys Rev Lett, 2008. 101(10): p. 108101.

Müller, K.W., et al., Rheology of semiflexible bundle networks with transient linkers. Phys Rev Lett, 2014. 112(23): p. 238102. 13.

- 14. Müller, K.W., C. Meier, and W.A. Wall, Resolution of sub-element length scales in Brownian dynamics simulations of biopolymer networks with geometrically exact beam finite elements. submitted 2015.
- 15. Cyron, C.J., et al., Equilibrium phase diagram of semi-flexible polymer networks with linkers. Europhys Lett, 2013. 102(3): p. 38003.
- Lieleg, O., M.M.A.E. Claessens, and A.R. Bausch, Structure and dynamics of cross-linked actin networks. 16. Soft Matter, 2010. 6(2): p. 218-225.
- 17. Urban, E., et al., Electron tomography reveals unbranched networks of actin filaments in lamellipodia. Nat Cell Biol, 2010. 12(5): p. 429-35.
- Broedersz, C.P., et al., Cross-link-governed dynamics of biopolymer networks. Phys Rev Lett, 2010. 105(23): p. 238101. 18.
- Lieleg, O., et al., Mechanics of bundled semiflexible polymer networks. Phys Rev Lett, 2007. 99(8): p. 088102. 19.

#### The high-frequency regime motivates an enhanced theoretical understanding of bundle networks

10<sup>7</sup>

Figure 5:

and low frequencies.

Rescaled rheological spectrum of cross-linked, bundled, semiflexible polymer networks.

Comparisons show excellent agreement between simulation and experiments at intermediate

# Simulation Governance: An Idea Whose Time Has Come

## *by* Barna Szabó szabo@wustl.edu

"That is why finite element modeling should never be confused with numerical simulation." There are substantial economic incentives to reduce reliance on physical testing and increase reliance on numerical simulation. The reasons for this are obvious: Testing is expensive and time consuming and the results of tests are tied to the specific conditions under which they were performed. Testing without a properly formulated plan about how the results will be interpreted and generalized makes no sense. The main points are discussed in the following.

## Simulation

Simulation is the imitative representation of the functioning of one system or process by means of the functioning of another. Here we consider the functioning of mechanical and structural systems and their imitative representation by mathematical models.

We view simulation as a transformation of one set of data **D** into another set **F** using the available background information and know-how **I**. In short hand:

## $(\mathbf{D}, \mathbf{I}) \rightarrow \mathbf{F}$

An important question that professional analysts must be able to answer is this: Are **D** and **F** such that they lie within the range of validity of the assumptions incorporated in a mathematical model? For example, in the classical beam model shear deformation is neglected. For what range of **D** is this permissible? How can we tell whether a particular **D** lies within range of validity of the model? What to do when **D** is outside of the range of validity of the model?

*Figure 1:* The main elements of numerical simulation

## **Numerical simulation**

The purpose of simulation is to predict **F**. However, owing to the complexity of the vast majority of practical problems, the best we can do is to find an approximation to **F** by numerical means, usually by the finite element method. We denote this approximation by  $\mathbf{F}_{num}$ . The main elements of numerical simulation are illustrated in *Figure 1*.

Numerical simulation raises the obvious question: Under what conditions are we justified in substituting  $F_{num}$  for F?

Let us assume that we have formulated a mathematical model and it is known that **F** exists and is unique. (F exists only if the quantities of interest are finite numbers). Note that **F** exists independently from the numerical method used for finding  $F_{num}$ . Furthermore, the numerical method must have the property that, as the number of degrees of freedom N is increased, the difference  $F - F_{num}$  decreases. In the finite element method N is typically increased by mesh refinement, increase of the polynomial degree of the elements, or both.

 $\label{eq:Fnum} \begin{array}{l} \textbf{F}_{num} \text{ cannot be close to } \textbf{F} \text{ if it changes} \\ \text{substantially with } \textbf{N}. \ \text{This is a necessary} \\ \text{condition for the acceptance of } \textbf{F}. \\ \text{Reporting } \textbf{F}_{num} \text{ without:} \end{array}$ 

(a) knowing that **F** is a finite number and (b)  $\mathbf{F}_{num}$  is substantially independent of N should never be acceptable. For details on how fast  $\mathbf{F}_{num}$  approaches **F** with respect to increasing N we refer to [1].



## Finite element modeling is not numerical simulation

The term finite element modeling refers to the practice of selecting elements from the finite element library of an FEA software product and constructing from those elements a numerical problem that is supposed to represent some physical reality. In the points where rigid elements are connected to an adherend the strain would be infinitely large in a mathematical model based on the theory of continuum mechanics. However a finite element solution will produce finite strains that change as the mesh is refined. In other words, the finite element solution would strongly depend on the choice of the mesh. Two analysts using different meshes would be more than likely to come up with very different answers.



A schematic representation of finite element modeling is shown in *Figure 2* where the question mark indicates that it is generally not clear what the underlying mathematical model is.

In our short hand notation:

 $(D,\,I) \to F_{num}$ 

Many practitioners of finite element modeling mistakenly believe that if two nodes of any combination of elements in a finite element library can be connected then the resulting assembly of elements will correspond to an approximation to a well-defined mathematical model.

The following example of a finite element model intended for simulating the mechanical response of an adhesive in a bonded joint illustrates this practice<sup>1</sup>:

"The method uses a gap the thickness of the adhesive, two rigid elements, and three zerolength spring elements between coincident nodes. One rigid element stretches from one adherend to a node at the center of the gap, while the second rigid element stretches from the other adherend to a coincident node also at the center of the gap..."

What is wrong with this approach? – It is not clear how rigid elements and zero length spring elements represent the mechanical response of an adhesive. The mathematical model is not defined, therefore it is not possible to estimate the difference  $\mathbf{F} - \mathbf{F}_{num}$ . In fact, if  $\mathbf{F}$  includes the normal and shear stresses on the interfaces between the adhesive and the adherends then  $\mathbf{F}$  does not exist. Therefore  $\mathbf{F}_{num}$  will be an approximation to a non-existent  $\mathbf{F}$ .

Practitioners of finite element modeling are often perplexed by "non-physical hot spots" observed at point constraints and at reentrant corners. These are manifestations of conceptual errors associated with finite element modeling.

A thoroughly documented example of wildly erroneous results produced by finite element modeling of a shell-solid connection is available in [2].

## **Correlation with experiments**

Suppose that an experiment is to be performed to test the veracity of predictions based on a mathematical model. We denote the measured data by  $F_{exp}$ . We are interested in the difference  $F - F_{exp}$ . However we have available  $F_{num}$  only. By adding and subtracting  $F_{num}$  we have:

 $\mathbf{F} - \mathbf{F}_{exp} = (\mathbf{F}_{num} - \mathbf{F}_{exp}) + (\mathbf{F} - \mathbf{F}_{num})$ 

This means that we are justified in relying on the first bracketed expression on the right if and only if it is shown by independent means that  $(\mathbf{F} - \mathbf{F}_{num})$  is smaller than the errors in the experimental measurements. This is a key technical requirement, called solution verification, which is a prerequisite for model validation [1].

Since **F** does not appear in finite element modeling, and, in fact it may not even exist, the predictive performance of finite element models cannot be tested. Therefore finite element modeling does not meet the technical requirements of verification and validation.

Figure 2: The scheme of "finite element modeling"

Numerical simulation is concerned with the formulation of mathematical models and the corresponding quantities of interest **F** which are approximated by numerical means. Finite element modeling, on the other hand, fails to distinguish between **F** and  $\mathbf{F}_{num}$  and hence does not meet the technical requirements of verification and validation. That is why finite element modeling should never be confused with numerical simulation.

## **Simulation Governance**

Simulation governance is the exercise of command and control over all aspects of numerical simulation [3], [4]. Reliance on predictions based on mathematical models is justified if and only if convincing experimental evidence is available demonstrating that the transformation  $(D, I) \rightarrow F$  yields predictions that are consistently confirmed by the outcome of physical experiments.

Simulation governance is concerned with the selection and adoption of the best available simulation technology, the formulation of mathematical models, the management of experimental data, the verification procedures, and the revision of mathematical models in the light of new information collected from physical experiments and field observations.

The key elements of simulation governance are verification, validation and uncertainty quantification (VVUQ) [1], [5].

Verification is concerned with the accuracy of the numerical solution of a mathematical model and encompasses code verification, data verification and solution verification. Whereas code verification is the responsibility of the code developer, data verification and solution verification are among the most important responsibilities of the users. Software products qualified to support simulation governance must provide the means users need to exercise those responsibilities. Validation is concerned with objective assessment of the predictive performance of mathematical models by comparing simulation results with the outcome of experiments, while accounting for the effects that uncertainties in (D, I) have on the quantities of interest **F**.

Uncertainty quantification is concerned with the stochastic aspects of **D**. In solid mechanics mathematical models are typically deterministic but the input data are stochastic. Therefore predictions based on mathematical models have to be stochastic.

## **Closing remarks**

With very few exceptions, physical testing is being conducted without a properly formulated plan for the generalization of the test results. Consequently the return on investment on testing programs is much smaller than it would be had testing been conducted under the rules of simulation governance.

For example, a great deal has been invested into the development of design rules for composite materials, yet the predictive performance of mathematical models conceived to support design and certification of structural components made of composite materials has not been satisfactory [6].

The available data **D** and background information I change over time. Therefore it is possible to improve the predictive performance of mathematical models over time. It is the responsibility of engineering management to establish a framework for simulation governance that includes systematic review and revision of simulation practices in the light of new information.

Finding a nearly optimal balance between physical testing and numerical simulation is a problem of resource allocation. This problem can be solved only if the software tools used for generalization of the test results meet the technical requirements outlined herein.

## References

- [1] *Szabó, B. and Babuška*, I. Introduction to Finite Element Analysis: Formulation, Verification and Validation. John Wiley and Sons, Ltd. Chichester, UK (2011).
- [2] Szabó, B., Babuška, I., Pitkäranta, J. and Nervi, S. The problem of verification with reference to the Girkmann problem. Engineering with Computers. Vol. 26, pp. 171-183 (2010).
- [3] *Szabó, B. and Actis, R.* Simulation governance: Technical requirements for mechanical design, Comput. Methods Appl. Mech. Engng., Vol. 249 252, pp. 158 168 (2012).
- [4] Simulation & Analysis Governance: A Strategy to Advance the Value of S&A. CIMdata, Inc., *Ann Arbor*, Michigan, April 2014.
- [5] *Oberkampf WL and Roy CJ.* Verification and Validation in Scientific Computing. Cambridge University Press, 2010.
- [6] *Hinton M.* Failure Criteria in Fibre Reinforced Polymer Composites: Can any of the Predictive Theories be Trusted? NAFEMS World Congress, Boston, 23rd-26th May 2011.

investment ... is much smaller than it would be ...under the rules of simulation governance."

"the return of

## Petascale Coupled Simulations of Real World's Complex Structures

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> Leading supercomputers offer the computing power of petascale, and exascale systems are expected to appear in the end of this decade [1]. Supercomputers with more than tens of thousands of computing nodes, each of which has many cores, cause serious problems in practical finite element software. Not only the time consuming hot spots of the

algorithms but also the entire algorithms must be well tuned and parallerized [2]. For example, K computer, a Japanese Petaflops machine consists of 88,128 processing nodes and 705,024 cores, and achieves peak performance of 10.5 Peta FLOPS. Latest HPC machines require the following three-layered parallelisms, i.e. (1) Speedup within core, (2) Parallelism in inter-node : Increase parallel efficiency in multicore calcuation considering memory band width, and (3) Parallelism in intra-node : Increase parallel efficiency in intra-node calculation considering intra-node communication speed.

Since 1997, we have been developing a unique open source parallel finite element software known as ADVENTURE [3-7], which enables very precise analyses of practical structures and machines using over 100 million to billions DOF mesh.

The parallel solution algorithm employed is the hierarchical domain decomposition





method (HDDM) [8,4] with balancing domain decomposition (BDD) [9,5,6] as preconditioner. Figure 1 illustrates the schematic analysis flow of the HDDM-BDD algorithm implemented in ADVENTURE\_Solid code. In addition, we have developed a generalized parallel IO system [4], a hierarchical domain decomposition module [4,7], and parallel and walkthrough visualization modules [4]. Since December 2002, 40,400 modules of the system have been downloaded by 8,540 registered users worldwide. Its commercial version named ADVENTURECluster [10] has also been widely adopted in automobile, E&E/ICT, heavy, space, material and construction industries, and was recognized as 2006 IEEE/ACM Gordon Bell finalist.

As one of various application problems, we have been studying seismic response and structural integrity evaluation of existing nuclear power plants (NPPs) attacked by strong earthquake exceeding design limit [5,11,12]. In such countries as Japan where earthquakes occur frequently, reliable and sufficient seismic proof design plays a key role in operating NPPs safely and stably. Especially, recent strong earthquakes having attacked several Japanese NPPs such as Niigataken-Chuetsu-Oki (NCO) earthquake with 6.8 Mw occurred on July 16, 2007 and Great East Japan Earthquake and Tsunami with 9.0 Mw occurred on March 11, 2011 recalled its practical importance seriously.

Figure 3: Core shroud and shroud inside





In conventional seismic design of NPPs, a variety of safety margins are embedded in various ways to take into account uncertainties in design and operation processes. However, it is still a big concern how strong earthquake existing NPPs can stand in reality. Thus we rely on constructing full scale and high fidelity three-dimensional finite element models of building, pressure vessels and internal structures with millions to billions DOF mesh, and on performing seismic response analyses.

*Figures 2 and 3* show the finite element models of boiling-water reactor (BWR). *Figure 4* shows a snapshot of the calculated Mises stress distributions around the stabilizer of reactor pressure vessel against NCO 2007 wave [11]. Using the latest version of ADVENTURE system on the K computer, we are now performing a precise investigation on how the Unit 1 of TEPCO's Fukushima Dai-ichi NPP facilities responded during 140 seconds to the Great East Japan Earthquake of 9.0 Mw. *Figure 5* shows its CAD model.

In addition to increasing model size for solving real world's complex-shaped structures and systems, strong demands are emerging on evaluation of their multi-physics behaviors. We have also being developing a parallel coupled simulation system for large-scale multiphysics problems. Our coupled simulation approach consists of the following three basic philosophies, i.e. (1) Partitioned Approach to use various kinds of existing solvers optimized for parallel computers such as ADVENTURE, (2) Fixed Point Iteration to improve accuracy and *Figure 4: Mises stress distributions around the stabilizer of reactor pressure vessel* 

robustness although added mass effects are still big issues for partitioned approaches, and (3) Parallel Coupling Tool named ADVENTURE\_Coupler to integrate two or more independent parallel solvers with only minimum modification to them. Among various iterative coupled algorithms in literature, we have selected some algorithms meeting the following three criteria :

(1) Robust convergence,

(2) Ability to treat each parallel solver as black box, and

(3) Easy and efficient parallelization.

Finally, Gauss Seidel, matrix free Newton-Krylov and Quasi-Newton methods have been selected [13] and implemented in the ADVENTURE Coupler [14]. The coupler realizes automatic construction of mapping relation between complex-shaped interface surfaces considering different mesh subdivision and different subdomain decomposition as schematically shown in Figure 6. The coupler offers parallel communication capability. In each parallel solver, some IO portions are just replaced with communication libraries. Thanks to them, a whole coupled simulation process can be fully parallelized. The coupler also takes care of interpolating physical variables between non-matching meshes, preserving conservation.

"The coupler offers parallel communication capability."



CAD model of Unit 1 of TEPCO's Fukushima Dai-ichi NPP facilities

## **References:**

- [1] *J. Dongarra et. al.* **The international exascale software roadmap.** International Journal of High Performance Computing Applications, 25, 3-60, 2011.
- [2] M. Papadrakakis G. Stavroulakis, A. Karatarakis. A new era in scientific computing : domain decomposition methods in hybrid CPU-GPU architectures. Computer Methods in Applied Mechanics and Engineering, 200, 1490-1508, 2011.
- [3] http://adventure.sys.t.u-tokyo.ac.jp/
- [4] S. Yoshimura, R. Shioya, H. Noguchi, T. Miyamura. Advanced general-purpose computational mechanics system for large scale analysis and design. Journal of Computational and Applied Mathematics, 149, 279-296, 2002.
- [5] *M. Ogino, R. Shioya, H. Kawai, S. Yoshimura.* Seismic response analysis of full scale nuclear vessel model with ADVENTURE system on the Earth Simulator. Journal of the Earth Simulator, 2, 41-54, 2005.
- [6] *T. Miyamura*. **Incorporation of MPCs into the BDD and its parallel implementation**. International Journal for Numerical Methods in Engineering, 69, 326-346, 2007.
- [7] K. Murotani, S. Sugimoto, H. Kawai, S. Yoshimura. Hierarchical domain decomposition with parallel mesh refinement for billions-of-DOF scale finite element analyses. International Journal of Computational Methods, 11/4, 1350061, 2014.
- [8] *G. Yagawa, R. Shioya*. **Parallel FE on massively parallel computer with domain decomposition**. Computer Systems in Engineering, 4, 495-503, 1994.



- [9] *J. Mandel*. **Balancing domain decomposition**. Communications on Numerical Methods in Engineering, 9, 233-241, 1993.
- [10] *H. Akiba, S. Yoshimura, H. Noguchi, et al.* Large scale drop impact analysis of mobile phone using ADVC on Blue Gene/L. Proceedings of IEEE/ACM Supercomputing' 06, CD-ROM, 2006.
- [11] S. Yoshimura, K. Kobayashi, H. Akiba, S. Suzuki, M. Ogino. Seismic response analysis of full scale boiling water reactor using three dimensional finite element method. Journal of Nuclear Science and Technology, 52/4, 546-567, 2015.
- [12] S. Yoshimura, M. Hori, M. Ohsaki. High-performance computing for structural mechanics and earthquake / tsunami engineering. Springer, to Appear.
- [13] S. Minami, S. Yoshimura. Performance evaluation on nonlinear algorithms with line-search for partitioned coupling techniques for fluid-structure interactions. International Journal for Numerical Methods in Fluids, 64/10-12, 1129-1147, 2010.
- [14] *S. Kataoka, S. Minami, H. Kawai, T. Yamada, S. Yoshimura.* **A parallel iterative partitioned coupling analysis system for large-scale acoustic fluid-structure interactions**. Computational Mechanics, 53/6, 1299-1310, 2014.

## Discrete Stability Challenge and the Discontinuous Petrov Galerkin (DPG) Method with Optimal Test Functions

## (Dedicated to Prof. Babuška on the Occasion of the Oncoming 90th Birthday)

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## bstract

We review the Babuška Theorem and the concept of discrete stability (inf-sup condition), and show how it led to the DPG method with optimal test functions.

Variational formulations. Well posedness. The (Petrov-) Galerkin method (1914,1959) starts with a variational problem for a boundary-value problem (BVP) (or a corresponding integral equation) which can be conciselv written in the abstract form:

$$\begin{cases} u \in U \\ b(u, v) = l(v) \quad v \in V. \end{cases}$$

Here U and V are energy (Hilbert) trial and test spaces, u is the solution, v stands for test functions, bilinear form b(u, v) represents the involved differential (integral) operators, and linear form l(v) represents the right-hand sides of the equations and boundary conditions (BC). In general, a BVP admits several variational formulations with different functional setting, i.e. energy spaces U, V [9]. When U = V, we speak about a symmetric functional setting in which case, the problem can be discretized with a Bubnov-Galerkin method. To this class belongs Principle of Virtual Work and various mixed formulations. If additionally form b is symmetric, b(u, v) = b(v, u), the problem is called symmetric. Nonsymmetric formulations include the *trivial* variational formulation, equivalent to the strong form of the equations and leading to least squares discretizations, and the ultra-weak variational formulation in which all derivatives are passed to test functions, and solution lives in the  $L^2$  trial space. For complex-valued problems (wave propagation, vibrations), energy spaces are complex, and we may choose to work with forms b(u, v) and l(v) that are antilinear in v. Each variational formulation leads to a different Finite Element (FE) method, although some are easier to discretize. Dependent upon the formulation and energy setting, convergence will take place in a *different norm*  $||u||_{U}$ .

The formalism of bilinear and linear forms became popular only in fifties with the rise of FE method. It provides not only a basis for analysis but also for coding. Already a half a century earlier (Hilbert, Fredholm, Banach), same problems were analyzed using the language of operators. Indeed, variational problem (0.1) can be written in the operator form,

$$Bu = l, \quad B: U \to V', \quad \langle Bu, v \rangle_{V' \times V} = (Bu)(v) = b(u, v), \quad u \in U, v \in V,$$

where the linear operator B takes values in the dual space V'. This is the essence of a variational problem in the language of operators. It goes without saying that b(u, v) and l(v)are continuous,

$$b(u,v)| \le M \|u\|_U \|v\|_V, \qquad |l(v)| \le \|l\|_{V'} \|v\|_V.$$

The continuity constant for form l(v) can be identified as the norm of l(v) in the dual space, whereas the continuity constant M can be identified as the norm of operator B.

Babuška -Nečas Theorem states that the variational problem is well posed, provided the bilinear form satisfies the inf-sup condition,

$$\sup_{v \in V, v \neq 0} \frac{|b(u, v)|}{\|v\|_V} \ge \gamma \|u\|_U \quad \Leftrightarrow \quad \|Bu\|_{V'} \ge \gamma \|u\|_U$$

and the right-hand side satisfies the compatibility condition:

(0.4)

(0.2)

(0.3)

(0.1)

$$l(v) = 0 \quad v \in V_0 := \{ v \in V : b(w, v) = 0 \quad \forall w \in U \}.$$

By the well-posedness, we mean that the solution exists, it is unique, and it depends continuously upon data. More precisely,

$$\|u\|_U \le \frac{1}{\gamma} \|l\|_{V'} \,. \tag{0.6}$$

A few comments are in place. The inf-sup condition<sup>1</sup> is equivalent to the condition that operator *B* is bounded below. Since time of Banach's dissertation (Closed Range Theorem), we all know that this is a *sine qua non* condition for the well-posedness of a linear problem. Do not dream thus about circumventing the inf-sup condition, please. In fact, as stated, Babuška -Nečas Theorem is a direct consequence of Banach Close Range Theorem (for continuous operators). Space  $V_0$  is the null space of the adjoint *B*' which, for a Hilbert space *V*, goes from *V* into *U*' and it is determined by b(u, v) in the same way as operator *B* by switching *u*, *v* with each other.

**Petrov-Galerkin method.** Babuška 's Theorem and discrete stability. The Galerkin method is obtained by replacing energy spaces U, V in (0.1) with finite dimensional trial and test subspaces:  $U_h \subset U$ ,  $V_h \subset V$  of equal dimension, dim  $U_h = \dim V_h$ . In simple terms, this means that we approximate both solution u and test functions v with linear combinations:

$$u(x) \approx u_h(x) := \sum_{i=1}^N u_i e_i(x), \qquad v(x) \approx v_h(x) := \sum_{j=1}^N v_j g_j(x),$$

where the unknown degrees-of-freedom (d.o.f.)  $u_i$  are to be determined, and the variational problem is to be satisfied for arbitrary coefficients  $v_j$ . If the test basis functions  $g_j$  coincide with the trial basis functions  $e_i$ , we have a Bubnov-Galerkin method; if they are different, we speak about the Petrov-Galerkin method. The approximate variational problem,

$$\begin{cases} u_h \in U_h \subset U\\ b(u_h, v_h) = l(v_h) \quad v_h \in V_h \subset V, \end{cases}$$

$$(0.7)$$

reduces to a system of *N* linear algebraic equations <sup>2</sup> with *N* unknowns. The use of different trial and test basis functions is natural in the case of a non-symmetric functional setting but it may be necessary in case of U = V as well.

The famous Babuška Theorem [1] postulates that spaces  $U_h$ ,  $V_h$  should be selected in such a way that the bilinear form  $b(u_h, v_h)$  satisfies the discrete equivalent of the inf-sup condition,

$$\sup_{v_h \in V_h, v_h \neq 0} \frac{|b(u_h, v_h)|}{\|v_h\|_V} \ge \gamma_h \|u_h\|_U$$

Not surprisingly<sup>3</sup>, the discrete problem is then well-posed, with the discrete stability condition,

$$\|u\|_{U} \le \frac{1}{\gamma_{h}} \|l\|_{V_{h}'}$$
(0.9)

and the following error estimate holds:

$$\frac{\|u - u_h\|_U}{\text{Galerkin error}} \leq \underbrace{\frac{M}{\gamma_h}}_{\text{stability constant best approximation error}} \underbrace{\inf_{w_h \in U_h} \|u - w_h\|_U}_{\text{best approximation error}}.$$
(0.10)

If the discrete stability constant stays bounded below,  $\gamma_h \ge \gamma_0 > 0$ , then  $M / \gamma_h \le M / \gamma_0$ , and we have the famous phrase:

#### (Uniform) discrete stability and approximability imply convergence.

A few important comments. The *best approximation error* (BAE) is controlled by the choice of trial basis functions  $e_i$ . Given any a-priori information about the solution, we select the trial functions in such a way that we can control the BAE. For example, in elasticity, in the case of a jump in elasticities across an interface, the corresponding stress vector is continuous across the interface but the strain tensor *is not*. Consequently, using  $C^i$ -continuous elements across such an interface makes little sense as we would have to approximate a discontinuous

<sup>&</sup>lt;sup>1</sup>Divide (0.4) by kul and take infimum in u to see it.

<sup>&</sup>lt;sup>2</sup> For a nonlinear problem, the equations are nonlinear.

<sup>&</sup>lt;sup>3</sup> A direct consequence of Babuška -Nečas Theorem specialized to the discrete setting.

function with continuous ones. By the same reasoning, we should try to match material interfaces with finite elements if within each element we use just polynomial shape functions. Otherwise, we attempt to approximate low regularity solution (jumps in strains) with smooth shape functions, a bad idea. Similarly, for Maxwell equations, if the dielectric constant jumps across an interface, the corresponding *normal* component of electric field E(x) is *discontinuous* across the interface. Using (globally) continuous elements to approximate such fields is a bad idea.

The continuous inf-sup condition *does not imply* its discrete counterpart. Indeed, specializing (0.4) to  $u_h \in U_h$ , we see that

$$\sup_{v \in V} \frac{|b(u_h, v)|}{\|v\|_V} \ge \gamma \|u_h\|_U \quad \neq \quad \sup_{v_h \in V_h} \frac{|b(u_h, v_h)|}{\|v_h\|_V} \ge \gamma \|u_h\|_U \tag{0.11}$$

The reason is clear, the supremum on the left is taken over an infinite dimensional space V whereas the supremum on the right only over the finite dimensional subspace  $V_h \subset V$ , and it may be much smaller. It becomes clear that the choice of discrete test basis functions  $g_i$  controls the discrete stability.

**Concept of optimal test functions.** In the standard Galerkin method, the basis functions *are assumed*. According to our discussion above, the trial basis functions are designed to control the BAE, whereas the test basis functions are supposed to control the stability, i.e. the discrete inf-sup condition. The *optimal test functions* [11]  $v_h = |v_{\delta u_h} \in V_h$  corresponding to a trial function  $\delta u_h$  realizes the supremum in the continuous inf-sup condition,

$$\sup_{v \in V} \frac{|b(\delta u_h, v)|}{\|v\|_V} = \frac{|b(\delta u_h, v_{\delta u_h})|}{\|v_{\delta u_h}\|_V}$$
(0.12)

It takes a bit of familiarity with Riesz Theorem, to show that

2

$$v_{\delta u_h} = R_V^{-1} B \delta u_h$$

(0.13)

where  $R_v: V \to V'$  is the Riesz operator, an isometric isomorphism, mapping test space V onto its dual. We call the operator  $T := R_v^{-1} B: U_h \to V$ , the *trial-to-test operator*. Obviously, T is injective; its range  $R(T) = T(U_h)$  is identified as the *space of optimal test functions*. It follows from the construction that, contrary to an hoc selected test space  $V_h$ , the use of optimal test functions guarantees the implication in (0.11). In other words, if the continuous variational problems is well posed, then so its Galerkin approximation with the optimal test functions with a discrete stability constant  $\gamma_h \ge \gamma$ . Formula (0.13), i.e. the inversion of Riesz operator, hides the solution of an additional, auxiliary variational problem,

$$\begin{cases} v_{\delta u_h} \in V \\ (v_{\delta u_h}, \delta v)_V = b(\delta u, \delta v) \quad \delta v \in V . \end{cases}$$
(0.14)

In the DPG method, a practical inversion of Riesz operator is made possible by utilizing two techniques. The first one comes from the use of variational formulations with *broken* (*discontinuous*) test spaces and *localizable test norms*. Computation of the test inner product *localizes* to computations on individual elements *K* from a given mesh  $T_h$ ,

$$(v,\delta v)_V = \sum_K (v_K,\delta v_K)_{V_K} \quad v = \{v_K\}_{K\in\mathcal{T}_h}, \, \delta v = \{\delta v_K\}_{K\in\mathcal{T}_h},$$

and the inversion of Riesz operator in (0.14) can be done *element-wise*. The second step consists of approximating the element version of (0.14) with a standard Bubnov-Galerkin method using an *enriched test space*. We will further explain it below. We mention also that we can take any well-posed variational formulation using standard test spaces  $H^{i}$ , H(curl), H(div), and "break" the test functions, i.e. replace the energy space with its broken equivalent. The price paid for the use of broken test spaces (localization) is the introduction of additional unknowns: fluxes and/or traces that live on the mesh skeleton (DPG is a hybrid method). The formulation with broken test spaces retains the well-posedness of the original formulation [10]. In the beginning, we used DPG with ultra-weak formulations only, later we applied it to the standard, classical formulation (primal DPG method), now we have realized that we can apply the DPG methodology to *any well-posed variational problem*.

A few comments are in place now. The main idea behind the DPG method is to *compute* rather than to assume test functions. The concept of our optimal test functions should not be confused with the optimal test functions of Barret and Morton [3]. Our trial-to-test operator is  $T^{DG}$ : =  $R_v^{-1} B$ , whereas Barret-Morton's operator is  $T^{MB}$ : =  $B'^{-1} R_U$  see the diagram below,

$$\begin{array}{cccc} U & \xrightarrow{B} & V' \\ R_U \downarrow & & \downarrow R_V \\ U' & \xleftarrow{B'} & V \sim V'' \end{array}$$

Computation of DG optimal test functions involves inversion of a self-adjoint, positive-definite Riesz operator  $R_v$  whereas computation of BM test functions involves inversion of transpose B'. Surprisingly perhaps, a special choice of test norm in DPG (scaled adjoint graph norm) leads in a limit to BM test functions, i.e. DPG provides practical means for computing BM test functions, see [5]. Finally, we mention that in case of trivial variational formulations where  $V = L^2$  ( $\Omega$ ), Riesz operator reduces to an identity, and the concept of optimal test functions leads to the standard least squares method.

**Minimum residual method and the mixed method interpretation.** Surprise or not, the concept of Petrov-Galerkin method with optimal test functions leads through back door to a minimum residual method. The argument is so simple that we dare to show it. We first introduce an "energy norm"<sup>4</sup>.

$$\|u\|_{E} := \|Bu\|_{V'} = \|R_{V}^{-1}B\|_{V} = \sup_{v \in V} \frac{|b(u,v)|}{\|v\|_{V}}.$$
(0.15)

If we replace the original norm  $||u||_U$  with the energy norm  $||u||_E$ , we learn that the corresponding continuity and inf-sup constant (that depend upon the choice of norms) are *both equal one*. Consequently, the Babuška Theorem delivers the following error estimate for the Petrov-Galerkin method with optimal test functions <sup>5</sup>,

$$\|u - u_h\|_E \le \underbrace{\frac{M}{\gamma}}_{=\frac{1}{1}=1} \inf_{w_h \in U_h} \|u - w_h\|_E = \inf_{w_h \in U_h} \|u - w_h\|_E$$

As  $u_h \in U_h$ , we have:

$$\|u - u_h\|_E = \inf_{w_h \in U_h} \|u - w_h\|_E = \|Bu - Bw_h\|_{V'} = \|l - Bw_h\|_{V'}.$$

In other words, solution  $u_h$  minimizes the residual  $r_h := l - Bu_h$  measured in the dual norm. Like it or not, the minimum residual method *is the most stable Petrov-Galerkin* discretization you can have. This explains a lot of important characteristics of the DPG method. In particular, the stiffness matrix is always hermitian and positive definite. Being a minimum residual method, DPG (like the Ritz method) does not suffer from any preasymptotic stability problems.

Finally, Cohen, Dahmen and Welper [8] realized that the minimization of residual is equivalent to the solution of the following mixed problem,

$$\begin{cases} u_h \in U, \ \psi \in V \\ (\psi, v)_V - b(u_h, v) = -l(v) \quad v \in V \\ b(\delta u_h, \psi) = 0 \qquad \delta u_h \in U_h \end{cases}$$
(0.16)

This is a strange mixed problem where one solves for the approximate solution  $u_h$  from the finite-dimensional trial subspace  $U_h$  and the Riesz representation <sup>6</sup> of the residual  $\psi = R_v^{-1} (Bu_h - l)$  from the infinite-dimensional space V.

**Practical DPG method. Enriched test space.** As mentioned above, the optimal test functions (and Riesz representation function  $\psi$ ) must be approximated. We approximate the mixed problem by replacing space V with a finite-dimensional *enriched space* 

 $\tilde{V}_h \subset V$ , dim  $\tilde{V}_h >> U_h$ ,

<sup>&</sup>lt;sup>4</sup>We should have called it rather the "residual norm". The bilinear form with test norm and the energy norm induced by the test norm becomes a duality pairing [4].

<sup>&</sup>lt;sup>5</sup>Notice that optimal test functions *do not depend* upon the choice of norm in U. <sup>6</sup>We called it initially "errror representation function".

$$\widetilde{u}_{h} \in U, \ \widetilde{\psi} \in \widetilde{V}_{h} \subset V$$

$$(\widetilde{\psi}, v)_{V} - b(\widetilde{u}_{h}, v) = -l(v) \quad v \in \widetilde{V}_{h}$$

$$b(\delta u_{h}, \widetilde{\psi}) = 0 \quad \delta u_{h} \in U_{h}$$

$$(0.17)$$

This leads to the saddle-point problem that has the following matrix form.

$$\begin{cases} G\psi & -Bu = -l \\ B^T\psi & = 0 \end{cases}$$
(0.18)

where  $\psi$  and u denote now vectors of d.o.f. for  $\tilde{\psi}$  and  $\tilde{u}_h$ , and G denotes the Gram matrix corresponding to the test inner product and the choice of the enriched space. The whole point of using broken test spaces lies in the fact that G is a block-diagonal matrix, and function  $\psi$  can be statically condensed to yield the final global system of equations in the form:

$$\underline{B^T G^{-1} B}_{\text{G stiffness matrix}} u = \underbrace{B^T G^{-1} l}_{\text{DPG load vector}} .$$

DPC

(0.19)

Functions  $u=B^{T}G^{-1} \delta u$  are the *approximate optimal test functions*, and the DPG system can be interpreted as a preconditioned (with  $G^{-1}$ ) least squares approximation to the system Bu = l where *B* is a rectangular matrix.

Finally, we can use the theory of mixed problem and concept of Fortin operators [13] to account for the error  $u_h - \tilde{u}_h$ ,  $\psi - \tilde{\psi}$  resulting from the approximation of the optimal test function and the Riesz representation  $\psi$  of the residual. Function  $\tilde{\psi}$  and its norm provide an excellent approximation for the element residual. As every minimum residual method, DPG comes with a built-in a-posteriori error estimate.

## DPG enables automatic adaptivity starting with coarse meshes and guarantees

**reliability.** As mentioned above, the DPG method guarantees stability for any trial spaces, does not suffer from preasymtotic stability problems and it comes with an a-posteriori error estimation built it. It provides a natural starting point for adaptive methods, including *hp*-adaptivity. The DPG technology can be applied to any wave propagation problem, including a variety of Maxwell problems (including metamaterials for which the standard methods fail), acoustics, elastodynamics, and a large class of coupled problems. With the DPG adaptive technology we aim at problems for which the adaptivity matters: high frequency and coupled problems with localized solutions, and low and medium frequency problems with singular solutions.





## Figure 1:

Gaussian beam problem,  $.\omega = 60\pi$ . First, 11th, 21st and 31st *hp*-adaptive mesh and the corresponding numerical solution (imaginary part of pressure)



The main concept of the adaptive DPG technology is illustrated in *Figure 1*. We use the ultraweak formulation for the 2D acoustics equations to simulate a Gaussian beam with over 45 wavelengths in the domain. We start with a mesh of just sixteen quadratic elements. With that resolution, of course, we are far away from satisfying the Nyquist criterion, and the corresponding solution is (on the scale of the exact solution) is practically zero. Nevertheless, even with this meaningless mesh and solution, we can start the adaptive process. The next three figures present three selected meshes from a series of 44 *hp*-adaptive meshes, with the corresponding solutions. The algorithm 'grows' the mesh with the resolution remaining very coarse in the part of the domain where the solution is close to zero. We use a simplified *hp*-strategy with *h*-refinements continued until a half-wave length is reached and then switching to *p*-refinements.

**Challenges.** There are many, and we mention a few only. We started 3D computations only a year ago and we quickly realized that speeding element computations is absolutely crucial. A brute force approach is to use parallel machines (element computations are embarrassingly parallel), more refined techniques may use tensorization of enriched test spaces, use of GPUs and optimized linear algebra packages. The work on iterative solvers and preconditioning has barely started [2]. There is very little theory for nonlinear problems although we have applied DPG to both compressible [7] and incompressible NS [14] equations.

The main challenge is perhaps best visible in context of singular perturbation problems where a success of DPG relies on selecting a test norm for which a/ the DPG method is not only automatically stable but also *robust*<sup>7</sup>, and b/ Inversion of the Riesz operator can be done approximately with a negligible error. The first condition is usually satisfied by the adjoint graph norm. Unfortunately, approximate inversion of the Riesz operator (0.14) is then not much easier than the solution of the original problem. Hence, different test norms must be used [12, 6]. Construction of such test norms requires a careful stability analysis for the problem at hand and it is not always accessible.

This is the second time, we attempt to attract readers of *Expressions* to the presented ideas. Those interested in state-of-the-art research on the subject, are cordially encouraged to attend the Second Workshop on Minimum Residual and Least Squares Methods that will take place at Delft University, on Nov. 2-4, 2015. More details about the workshop can be found at:

## http://www.dpg-ls-workshop.nl

<sup>7</sup> Inf-sup constant  $\gamma$  is *uniform* in perturbation parameter.

#### **References:**

- [1] *I. Babuška*. Error-bounds for finite element method. Numer. Math, 16, 1970/1971.
- [2] A.T. Barker, S.C. Brenner, E.-H. Park, and L.-Y. Sung. A one-level additive Schwarz preconditioner for a discontinuous **Petrov–Galerkin method**. Technical report, Dept. of Math., Luisiana State University, 2013. http://arxiv.org/abs/1212.2645.
- [3] *J.W. Barret and K.W. Morton.* Approximate symmetrization and Petrov-Galerkin methods for diffusionconvection problems. Comput. Methods Appl. Mech. Engrg., 46:97–122, 1984.
- [4] T. Bui-Thanh, L. Demkowicz, and O. Ghattas. Constructively well-posed approximation methods with unity inf-sup and continuity. Math. Comp., 82(284):1923–1952, 2013.
- [5] J. Chan, J. Gopalakrishnan, and L. Demkowicz. Global properties of DPG test spaces for convection-diffusion problems. Technical Report 5, ICES, 2013.
- [6] J. Chan, N. Heuer, Tan Bui-Thanh B., and L. Demkowicz. A robust DPG method for convection-dominated diffusion problems II: Adjoint boundary conditions and mesh-dependent test norms. Comput. Math. Appl., 67(4):771–795, 2014.
- [7] Jesse Chan. A DPG Method for Convection-Diffusion Problems. PhD thesis, University of Texas at Austin, July 2013.
- [8] A. Cohen, W. Dahmen, and G. Welper. Adaptivity and variational stabilization for convection-diffusion equations. ESAIM Math. Model. Numer. Anal., 46(5):1247–1273, 2012. see also Technical Report 2011/323, Institut fuer Geometrie und Praktische Mathematik.
- [9] L. Demkowicz. Various variational formulations and Closed Range Theorem. Technical report, ICES, January 15–03.
- [10] L. Demkowicz, C. Carstensen, and J. Gopalakrishnan. The paradigm of broken test functions in DPG discretizations of elliptic second–order PDEs. 2015. in preparation.
- [11] L. Demkowicz and J. Gopalakrishnan. A class of discontinuous Petrov-Galerkin methods. Part II: Optimal test functions. Numer. Meth. Part. D. E., 27:70–105, 2011. See also ICES Report 9–16.
- [12] *L. Demkowicz and N. Heuer.* Robust DPG method for convection-dominated diffusion problems. SIAM J. Num. Anal, 51:2514–2537, 2013. see also ICES Report 2011/13.
- [13] J. Gopalakrishnan and W. Qiu. An analysis of the practical DPG method. Math. Comp., 83(286):537–552, 2014.
- [14] *Nathan Roberts*. A Discontinuous Petrov-Galerkin Methodology for Incompressible Flow Problems. PhD thesis, University of Texas at Austin, August 2013.

## STRUCTURAL ANALYSIS WITH THE FINITE ELEMENT METHOD LINEAR STATICS VOLUME 2: BEAMS, PLATES & SHELLS



**Eugenio Oñate** Springer & CIMNE, 2013

ISBN: 978-1-4020-8743-1, 864 pages, hard cover, 94,95 € (List Price).

Contents: Foreword; Preface; 1. Slender Plane Beams. Euler-Bernoulli Theory; 2. Thick/Slender Plane Beams. Timoshenko Theory; 3. Composite Laminated Plane Beams; 4. 3D Composite Beams; 5. Thin Plates. Kirchhoff Theory; 6. Thick/Thin Plates. Reissner-Mindlin Theory; 7. Composite Laminated Plates; 8. Analysis of Shells With Flat Elements; 9. Axisymmetric Shells; 10. Curved 3D Shell Elements and Shell Stiffners; 11. Prismatic Structures. Finite Strip and Finite Prism Methods; 12. Programming the Fem For Beam, Plate and Shell Analysis in Mat-fem; Appendices A-I; References; Author Index, Subject Index.

This is the second volume on the Finite Element (FE) method for linear static structural analysis. The first volume (reviewed in an earlier issue of IACM Expressions) deals with rods (longitudinal deformation) and 2D and 3D solids. The present volume covers the FE analysis of beam, plate and shell structures, with an emphasis on structures made of composite materials. This is an advanced undergraduate textbook for engineering students, and has emerged (in its Spanish version) from the notes of a course taught by the author at the Technical University of Catalonia (UPC). The background required from the reader is the standard knowledge acquired in basic mathematics and engineering courses studied in the first years of engineering schools. A nicely written Foreword by Carlos Felippa points out the special features of the book.

The book roughly comprises four parts: chapters 1-4 on beams, chapters 5-7 on plates, chapters 8-11 on shells, and chapter 12 on programming aspects. The software MAT-Fem discussed in chapter 12 can be freely downloaded from the web. The book ends with a sequence of appendices on various technical subjects, a rich bibliography, and very detailed subject and author indices.

This is an excellent textbook for engineering students. Moreover, as far as I am aware, this is the most complete treatise of the subject existing today, by far wider and more up to date than other books covering FE structural analysis. As the case is for volume 1, the book is pleasant to read, with a logical structure that makes it easy for the reader to find what she is looking for, and is full of illustrations (made in the simple clear style of Zienkiewicz).

Most of the chapters discuss FE analysis associated with a certain structural theory, e.g. Bernoulli-Euler beam, Timoshenko beam, Kirchhoff plate and Reissner-Mindlin plate, and the corresponding shell theories. In each case the theory is explained first in detail, before the FE formulation and specific elements are discussed. This makes the book self-contained, and emphasizes the fact that there is always a mechanical theory behind

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any FE analysis, and that the user of the FE method must understand it sufficiently well, in addition to understanding the computational part of the analysis.

Slight inaccuracies are present in parts of the text discussing mechanical theories. In the Bernoulli-Euler beam theory (Section 1.2), the lateral normal stresses, not strains, should be assumed to be zero ( $\sigma_z = \sigma_y = 0$ ). The lateral strains are actually nonzero due to the Poisson effect. In the Saint Venant torsion theory, the "warping effect" is the bulging of the cross section, which does



not remain a plane, namely there is a nonzero axial displacement which is a function of the cross-sectional coordinates, in contrast to the case of circular cross sections. In Section 4.3, however, "warping effects" refer to nonzero axial strains and stresses due to torsion when warping is constrained, and the Saint Venant assumption of free warping is thus said to state that there are no warping effects. Of course, this is just a matter of terminology, but one which may confuse a reader who has been exposed to the Saint Venant theory before, and who may be surprised to read here that a bar with a solid cross section has no "warping effects." A second edition of this book should do justice with these slight inaccuracies.

Chapter 8, on shells as a collection of flat elements, includes a number of color figures that show state-of-the-art applications of FE structural analysis. See *Figs. 1-3*, which describe the analysis of a car body, of an inflatable pavilion structure and of a parachute, respectively.

The discussion of FE formulations and specific elements for beams, plates and shells is comprehensive, and includes, in addition to the classical material, a few non-standard features, which cannot be found in most other books. Worth mentioning, in particular, are the following:

- A thorough discussion of *locking* with all its forms, for beams, plates and shells, and of remedies for locking.
- Introduction of *Rotation-free elements* for beams, plates and shells.
- A thorough discussion of the analysis of *composite laminated structures*, including *Zigzag theories* for composite beams, plates and shells, and elements devised for them, as well as modeling of *delamination*.
- Detailed discussion of *both degenerated elements* (namely structural elements obtained by degenerating the 3D elasticity formulation) *and theory-specific elements* (namely elements obtained directly for a certain mechanical theory).
- Discussion of "*folded structues*," the singularity associated with them and ways to prevent such singularity.
- Discussion (although somewhat brief) on *advanced topics* such as adaptive modeling and isogeometric shell analysis.

**Figure 2:** FE analysis of an inflatable pavilion, and the real-life structure. This is Fig. 8.45 taken from the book





## Figure 3:

FE analysis of a parachute, modeled with 3-noded membrane triangles. This is Fig. 8.48 taken from the book Locking is explained in a clear and comprehensive manner. For example. Section 2.4 shows in a simple way the effect of shear locking in a Timoshenko element when the beam is very slender, and Section 2.5 looks at the same effect from an algebraic viewpoint. Remedies discussed here include reduced/selective integration, different order interpolation for displacements and rotations, and the assumed transverse shear strain (B-bar) approach. A large number of example problems are solved in detail.

The discussion on *rotation free* elements appears in the context of





said in one of his recent lectures: "Those of you who have ever coded a general  $C^1$  element will never forget it."

Zigzag theories are relatively recent mechanical theories for composite laminated beams, plates and shells that overcome the inconsistency inherent in the classical composite laminate theory with 3D elasticity. After the background and main idea are first explained in Chapter 3, the author concentrates on the so-called Refined Zigzag Theory (RZT) of Tessler et al., develops

*Figure 4:* a suitable element, discusses shear locking and convergence, and describes a large *Two types of* sequence of numerical experiments. I believe that this important material is not covered by any other book on FE analysis.

This figure appears in the book as in the book as Fig. 5.25, p. 275
 Not many books discuss such a wealth of elements for beams, plates and shells: both classical and recently devised, both with and without the effect of shear deformation, both degenerated and theory-specific, both conforming and non-conforming. Moreover, many of these elements are compared with each other in this book, both theoretically and numerically, so as to provide the reader with guidelines on choosing the most appropriate element in each case.

In summary, this is an excellent book on linear static FE structural analysis, and is apparently the most complete treatise of the subject existing today. Its scope is almost encyclopedic in nature. It can serve nicely both as a textbook for an engineering advanced undergraduate or graduate course, and as a reference book for practitioners.



Two types of rotation-free Kirchhof plate elements. This figure appears in the book as Fig. 5.25, p. 275



## **Polish Association for Computational Mechanics**

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**Figure 1:** Prof. Krzysztof Wilmański (1940 – 2012)

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## International Conference on Continuous Media with Microstructure

http://www.cmwm.put.poznan.pl/

The 2<sup>nd</sup> International Conference on Continuous Media with Microstructure (CMwM2015), an ECCOMAS Special Interest Conference, took place on

2 - 5 March 2015 at the conference centre in Łagów, Poland. The conference was organized by the Polish Academy of Sciences, Poznan University of Technology, Berlin University of Technology, and the Polish Association for Computational Mechanics.



The CMwM2015 conference was dedicated to the memory of Prof. Krzysztof Wilmański (*Figure 1*) – an outstanding scientists of international reputation, and brought together many of his friends and colleagues, who eagerly accepted the invitation of the conference chairpersons Bettina Albers (TU Berlin) and Mieczysław Kuczma (Poznan UT).

The CMwM2015 was a conference with an intimate atmosphere, attended by nearly 40 scientists from Brazil, Czech Republic, Estonia, Georgia, Germany, Italy, Poland, Russia, and the USA, who gave 35 presentations (*Figures 2 and 3*). The general lectures were delivered by:

- Tadeusz Burczyński, Intelligent optimization of media with microstructure
- *Carlo Giovanni Lai*, Measurement of damping ratio spectra in soils from the exact solution of Kramers-Krönig equations of linear viscoelasticity
- I-Shih Liu, A mixture theory of porous media and some problems of poroelasticity
- Martin Ostoja-Starzewski, Continuum mechanics beyond the second law of thermodynamics
- *Jörg Schröder*, A FE2-homogenization scheme for the analysis of product properties of two-phase magneto-electric composites
- David Smeulders, Electrokinetic experiments in porous media for energy applications

Figure 2: (from left to right) Przemysław Litewka, Ingo Müller, Tadeusz Burczyński, Bettina Albers, Tomasz Łodygowski, Paweł Wilmański & Mieczysław Kuczma during the opening session



Figure 3: Participants of CMwM2015



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The U.S. Association for Computational Mechanics continues to grow synergistically and expand its activities in various directions. In December 2014, the USACM Executive Committee approved the establishment of **USACM Technical Thrust Areas (TTAs)**.

The primary rationale behind this is to provide a structured approach to the various technical areas reflected in the current research trends and priorities in the national and international computational and engineering sciences landscape. It is anticipated that each TTA will sponsor workshops and thematic conferences and help organize minisymposia at the national congresses. They will also maintain a presence on the USACM website. We anticipate that the TTA's will help fortify multiple thrust areas in the computational mechanics community within USACM.

The chosen thrust areas include:

(i) Novel Methods in Computational Engineering and Sciences, (ii) Isogeometric Analysis, (iii) Multi-Scale, Multi-functional Materials and Structures, (iv) Uncertainty Quantification and Probabilistic Modeling, (v) Computational Fluid Dynamics and Fluid-Structure Interaction, (vi) Nanotechnology and Lower Scale Phenomena, (vii) Biological Systems, (viii) Manufacturing and Materials Processing, (ix) Mathematical Methods in Computational Engineering & Sciences, and (x) Large Scale Structural Systems and Optimal Design. The USACM Executive Council anticipates active participation of the community in these efforts.

USACM has continued to support travel for students and post-doctoral researchers to attend the World Congress on Computational Mechanics as well as the U.S. National Congresses. In July of 2015, 26 students were granted partial travel support to attend the 11th World Congress on Computational Mechanics in Barcelona.

This summer, a total of 60 students and postdoctoral fellows will have received some travel through USACM and the Army High Performance Computing Research Center at Stanford University. (The AHPCRC generously sponsors the student poster session at USNCCM13).

The following conferences and workshops that were held last year include:

- a. IGA 2014: Isogeometric Analysis: Integrating Design and Analysis, January 8-10, 2014, Austin, TX
- MMVMB II: Multiscale Methods and Validation in Medicine and Biology II, Biomechanics and Mechanobiology, February 13-14, 2014, Berkeley, CA
- c. USACM/IUTAM Symposium on Connecting Multiscale Mechanics to Complex Material Design, May 13-16, 2014, Evanston, IL
- d. USACM Workshop on Meshfree Methods for Large-Scale Computational Science and Engineering: Theory and Applications of Galerkin and Collocation Methods, October 27-28, 2014, Tampa, FL
- e. 4th International Congress on Material Modeling, May 27-29, 2015, Berkeley, CA

Looking ahead, the following will be held in the next year. These will be coordinated by individual TTA's and we anticipate many more as a result of the establishment of the TTAs.

- i. Nonlocal Models in Mathematics, Computation, Science, and Engineering, October 26-28, 2015, Oak Ridge National Laboratories, Tennessee
- MMVMB III: Multiscale Methods and Validation in Medicine and Biology II, Biomechanics and Mechanobiology, February 25-26, 2016, Los Angeles, CA
- iii. IUTAM Symposium on Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions, June 6-8, Baltimore, MD ●

## 4th International Conference on Material Modeling Berkeley, California

Over 200 researchers from 31 countries attended the 4th International Conference on Material Modeling in Berkeley, CA,

**May 27-29, 2015**. The conference was held on the campus of the University of California, Berkeley, and sponsored by USACM. The aim of the ICMM conference was to bring together researchers from the various fields of material modeling and material characterization and to cover essentially all aspects of material modeling.

Five parallel sessions were held over the three days in the following areas:

- nonlinear elasticity and viscoelasticity;
- plasticity and viscoplasticity;
- strain gradient & nonclassical approaches,
- atomistic to continuum transitions,
- micro- and nano-scale modeling of hcp alloys;
- nanomechanics;
- phase-transforming materials;
- multiscale modeling;
- granular materials and particle systems;
- polymeric materials;
- biomaterials;
- electronic materials;
- multiferroic materials;
- creep, damage, fracture and fatigue;
- experimental identification and material characterization;
- composites;
- and dislocation dynamics.

Organizers of the conference were P. Papadopoulos and S. Govindjee (Co-Chairs) from the University of California, Berkeley and A. Betram, from University of Magdeburg. This conference is the fourth in the ICMM series. The first ICMM took place in 2009 in Dortmund, Germany; the second in 2011 in Paris, France; the third in 2013 in Warsaw, Poland. ICMM5 is scheduled for June 2017 in Rome.



Figure 1: Participants at ICMM4 Dinner



Figure 2: Organizers: S. Govindjee and A. Bertram

## USACM Upcoming Events

- 13th U.S. National Congress on Computational Mechanics, San Diego, California, July 27-30, 2015; http://13.usnccm.org
- Nonlocal Models in Mathematics, Computation, Science, and Engineering, Oak Ridge National Laboratories, Tennessee, October 26-28, 2015; http://nlmcse.usacm.org/





## ACME-UK 2015 Conference Final Report

The Association of Computational Mechanics in Engineering (ACME) in the United Kingdom was founded in March 1992 with the purpose of promoting research in Computational Mechanics in the UK and establishing formal links with similar organisations across Europe and worldwide. The Association is affiliated with the European Community of Computational Methods in Applied Sciences (ECCOMAS) and the International Association for Computational Mechanics (IACM). The principal activity of ACME involves the organisation of an annual two-day Conference focussed on the latest developments and research trends in the field of Computational Mechanics. The Conference is particularly orientated towards encouraging young scientists in the field to present their current research at both Doctoral and Post-Doctoral levels. The Conference is therefore a unique forum to foster ideas, enable new multidisciplinary research approaches and establish collaborative research links, helping to build strong research networks within the UK and at an international level.

## http://www.swansea.ac.uk/engineering/research/acme2015



This year, the 23rd Edition of the ACME Conference has returned to Swansea University, where it was inaugurated in 1993. The Conference was held in the "Zienkiewicz Centre for Computational Engineering", College of Engineering, Swansea University, from the 8th to 10th April 2015. As it is well-known, since the pioneering work of Prof. O. Zienkiewicz in the 1960s, this Research Centre has accumulated a longstanding prestige in this field of science which has helped the city of Swansea to be recognised as the host for a world leading Centre of Research. The Conference was sponsored by the College of Engineering at Swansea University, the Institute of Mathematics and Its Applications (IMA), the Zienkiewicz Centre for Computational Engineering

(ZCCE) at Swansea University, the National Research Network in Advanced Engineering and Materials (NRN) and the Society for Industrial and Applied Mathematics (SIAM).

The Conference was preceded by the **4th ACME School** on the 8th of April, which focussed on the theme of *"Low or high order: this is the questions!* (*To p or not to p*)". With more than 100 attendees, four presentations were delivered by **Prof. K. Morgan, Dr. A. J. Gil, Dr. R. Sevilla** and **Dr. P. D. Ledger** as part of the School, taking advantage of the local expertise. The Conference was extremely successful and was attended by **142 delegates, from 12 different countries and 32 different institutions**. 99 four page papers were presented within the Conference, resulting in a Book of Proceedings of outstanding quality. Presentations were distributed among four parallel sessions, including a wide spectrum of research



topics, namely, solids mechanics, fluids dynamics, mesh generation, stochastics, composites, optimisations, advanced applications, coupled problems and fracture, to name but a few. All the presentations were of great quality, very well attended and chaired by experts in the field as part of the Local Scientific Committee.

In addition, the Conference counted as invited Keynote Speakers with four of the greatest scientists in the field, namely **Prof. J. Peraire** (Massachusetts Institute of Technology), **Prof. R. Löhner** (George Mason University), **Prof. L. Formaggia** (Politecnico di Milano) and **Prof. J. Schröder** (Universität Duisburg Essen). The organisers are extremely grateful to them for finding the necessary spare time in their extremely busy agendas in order to come to Swansea and for inspiring the next generation of computational mechanicians with their awe-inspiring talks.

Regarding entertainments, in the evening prior to the beginning of the Conference, a Welcome Cocktail was organised in the Waterfront National Museum, where all delegates had the opportunity to early register and enjoy some of the best views of the Marina in Swansea, whilst savouring some typical wines and canapés. The Banquet of the Conference was held at Swansea Marriott Hotel, in the evening of the first day, where delegates could enjoy some of the wonders of the local Welsh cuisine, such as Welsh lamb, whilst being entertained by the Swansea Male Choir, who sang some pieces of his outstanding repertoire.

As a closure to the Conference, four awards were given to the best contributions presented. The ACME Best PhD paper award was given to **Mr. Dirk Ekelschot**, the ACME Best Post-Doctoral paper award was given to **Dr. Chun Hean Lee**, the NRN award was given to **Dr. Sussane Clauss** and the SIAM Best PhD paper award was given to **Mr. Rogelio Ortigosa**. In addition, Mr. **Lucas Franceschi** was the winner of the Best Research Image Competition.

The organisers would like to thank Prof. Carlo Sansour and the entire ACME-UK Executive, for giving us the opportunity to organise the 23rd ACME-UK Conference at Swansea. We hope that the standards of this Edition have been, at least, at the level of previous editions .... and that hopefully, we have managed to beat them!





Dr. Antonio J. Gil and Dr. Rubén Sevilla ACME-UK 2015 Conference Chairmen



## French Computational Structural Mechanics Association

## **CSMA Prizes**

Every year CSMA rewards the best two PhD thesis of the year. For the 2014 edition, the "CSMA prize comitee has examined 19 applications. The two awardees are Robin BOUCLIER and Nicole SPILLANE. Nicole SPILLANE is designated as the CSMA candidate for the ECCOMAS award for the best Phd theses in 2014



## PhD title:

## tle: Isogeometric locking-free NURBS-based solid-shell elements for nonlinear solid mechanics



## Laboratory: LaMCoS Laboratory, Lyon

Supervisors: Alain Combescure and Thomas Elguedj The goal of the PhD is to extend the IsoGeometric Analysis to the solid-shells in order to allow to calculate thin structures using 3D solid elements, involving only displacements as degrees of freedom. However, the NURBS framework does not enable to solve directly the problem of locking which highly deteriorates the convergence of the solution. Robin has proposed a mixed formulation from which it has been possible to derive the equivalent B projection. From a

theoretical point of view, this strategy constitutes the most important result of his work: a systematic method to construct a consistent B projection is to first a mixed formulation. With regards to the implementation, the main idea to treat locking of the solid-shell elements has been to modify the average of the strain and stress components across the thickness of the shell. Hourglass control has also been added to stabilize the element in particular situations. The resulting element is of good quality for low-order approximations and coarse meshes: the quadratic version seems to be more accurate than basic NURBS elements of order 4. The proposed method leads to a global stiffness matrix of small size but full. This problem is inherent in NURBS. It has been limited here by using a local least squares procedure to approach the B projection. Finally, the mixed element has been successfully extended to geometric non-linearity, which reflects the ability of the methodology to be used in complex simulations. *Current situation:* Robin holds a post-doctoral fellow position within the ANR project "ICARE" : Generalized interfaces and non-intrusive coupling at Université de Toulouse (France), Clément Ader Institute (ICA) - Toulouse Mathematics Institute (IMT) (Mixed research unit CNRS 5219).



## Nicole SPILLANE

PhD title: Robust domain decomposition methods for symmetric positive definite problems.

Laboratory:Jacques Louis Lions Laboratory, Paris and Michelin, Clermont FerrandSupervisors:Frédéric Nataf and Patrice Hauret

The objective of this thesis is to design domain decomposition methods, which are robust even for hard problems that arise when simulating industrial or real life objects. For instance one particular challenge, which the company Michelin is faced with, is the fact that tires are made of rubber and steel, which are two materials with very different behavior laws. With classical domain decomposition methods, as soon as the partition into subdomains does not accommodate the discontinuities between the different materials, convergence deteriorates. For three popular domain decomposition methods (Additive Schwarz, FETI and BDD) Nicole has proved that by solving a generalized eigenvalue problem in each of the subdomains she can identify automatically which are the modes responsible for slow convergence. In other words she can divide the original problem into two sub-problems: the first one where we can guarantee that the domain decomposition method will converge quickly and the second where we cannot. The final idea is to apply projections to solve these two problems independently (this is also known as deflation): on the first we apply the domain decomposition method and on the second (we call it the coarse space) we use a direct solver, which we know, will be robust. Nicole guarantees theoretically that the resulting two level solver is robust. The other main feature of her algorithms is that they can be implemented as black box solvers meaning that heterogeneous materials is only one type of difficulty that they can identify and circumvent.

*Current situation:* Nicole holds a postdoctoral position at the Center for Mathematical Modeling (CMM) of the Universidad de Chile in Santiago where she is pursuing her work on Domain Decomposition.

## CSMA selected PhD thesis for the ECCOMAS Olympiads 2014

Omar Bettinotti, Anthony GIACOMA & Fan XU were selected to represent CSMA at the ECCOMAS Olympiads 2015 during the Young Investigators Conference 2015, 20-23 July in Aachen, Germany.

## **Omar BETTINOTTI**

#### PhD title: A weakly-intrusive multi-scale Substitution method in explicit dynamics Supervisors: Olivier Allix, LMT Cachan

This work describes the development and implementation of the proposed Finite Element weaklyintrusive coupling method for the simulation of impact tests on composite structures. Some of the most recent coupling technologies have been deeply investigated with the implementation in Matlab prototypes, in order to understand potentialities and issues and also to collect reference results. Then, a new methodology is introduced with studies of accuracy, stability and efficiency through Matlab prototypes and verifications in comparison with the reference coupling methods. Finally, the implementation of the methodology inside the existing commercial software Abaqus is described and the related features are discussed.

Current situation: Omar holds Software Developer position at Dassault Systemes - Simulia

## **Anthony GIACOMA**

## PhD title: Efficient acceleration techniques for nonlinear analysis of structures with frictional contact

*Supervisors:* **David Dureisseix and Anthony Gravouil, LaMCoS Laboratory, Lyon** In this dissertation, model reduction methods (both a posteriori and a priori approaches) are deployed i n order to implement efficient numerical methods to solve frictional contact problem in the finite element framework. First, small perturbations hypothesis with a quasi-static evolution are assumed. Then, reducibility of some frictional solutions is emphasized and discussed using the singular value decomposition. In addition, a scale separability phenomenon is enlightened. Then, the non-linear large time increment method (LATIN) is introduced. Secondly, an accelerated LATIN method is suggested by drawing an analogy between previous scale separability observations and the non-linear multigrid full approximation scheme (FAS). This accelerated non-linear solver relies essentially on the a posteriori model reduction approach. A precomputation strategy for modes relying on surrogate models is also suggested. Next, the proper generalized decomposition (PGD) is used to implement a nonlinear solver relying fundamentally on an a priori model reduction method. Finally, some extensions are given to assign parametric studies and to take into account an additional non-linearity such as elastoplastic constitutive laws. *Current situation:* Anthony holds Research Engineer position at Software Developer ANSYS

## Fan XU

PhD title: Numerical study of instability patterns of film film-substrate systems Supervisors: Michel Potier-Ferry, LEM3, Metz & Salim Belouettar, CRP Henri Tudor, Luxembourg This thesis proposes a whole framework to study the film/substrate buckling problem in a numerical way: from 2D to 3D modeling, from classical to multi-scale perspective. The main aim is to apply advanced numerical methods for multiple-bifurcation analyses to various film/substrate models, e specially focusing on post-buckling evolution and surface mode transition. The models incorporate the Asymptotic Numerical Method (ANM) as a robust path-following technique and bifurcation indicators well adapted to the ANM to detect a sequence of multiple bifurcations and the associated instability modes on their post-buckling evolution path. The ANM gives interactive access to semi-analytical equilibrium branches, which offers considerable advantage of reliability compared with classical iterative algorithms. Besides, an original nonlocal coupling strategy is developed to bridge classical models and multi-scale models concurrently, where the strengths of each model are fully exploited while their shortcomings are accordingly overcome. Discussion on the transition between different scales is provided in a general way, which can also be seen as a guide for coupling techniques involving other reduced-order models. Lastly, a general macroscopic modeling framework is developed and two specific Fourierrelated models are derived from the well-established classical models, which can predict the pattern formation with much fewer elements so as to significantly reduce the computational cost. Current situation : Fan holds a PostDoc position in Computational Solid Mechanics at LEM3. He works on Multi-scale modeling for instabilities in film/substrate by Fourier series and on 3D finite strain FE modeling of film/substrate with ANM accounting for hyperelastic material laws.













Figure 1: General assembly meeting



Figure 2: Special lecture given by Professor Norio Takeuchi in the JSCES Symposium 2015 The sixth assembly meeting of JSCES was held at Muza Kawasaki Symphony Hall, Kawasaki, Japan, on May 22nd, 2015 (*Figure 1*).

Both the operating and financial review for the previous fiscal year and the operation and financial plan for this fiscal year were reported in this meeting. After the assembly meeting, the JSCES's 20th Anniversary Planning and Management Committee presented the operating plan of the 20th Anniversary Scholarship for Young Investigators and called for making donations to the scholarship. The general idea of the scholarship is to promote young society members to attend WCCMs or IACM special interest conferences and then activate those members furthermore in international activities. The number of scholarship winners is one or two per a year with a prize of 100 thousand yen each.

The deliberation in the assembly was followed by a special lecture given by Prof. Norio Takeuchi of Hosei University, the former president of JSCES, who presented a talk entitled "Past, Present and the Future of the Computational Mechanics of Discontinua" (*Figure 2*). The presentation started with a description of changes in the modeling and numerical methods for simulating discrete phenomena, such as distinct element method (DEM) and discontinuous deformation analysis (DDA), along with a brief story on the rigid bodies – spring model (RBSM) developed by Prof. T. Kawai, which became a key model in the development of the lecturer's hybrid-type penalty

method (HPM). Then, he explained the systematization of these discrete element models and suggested in his conclusion a necessity of multistage failure simulations, which enables us to analyze a phenomenon from continuum phase to discontinuum phase in a single seamless calculation.

## Figure 3:

Group shot of some JSCES's Board Members and recipients of The Fellowship Award, The JSCES Achievement Award, Kawai Medal, Shoji Medal, Technology Prize, Outstanding Paper Award and Young Researcher Paper Award **First row from left:** Prof. D. Isobe, Dr. Y. Yoshida, Prof. M. Kawahara, President S. Koshizuka, Dr. M. Shoji, Dr. M. Okuda, Dr. K. Ishii and Mr. M. Tsukino. **Second row from left:** Prof. M. Kurumatani, Mr. K. Nishiguchi, Prof. S. Okazawa, Mr. Y. Umezu, Mr. N. Yamasaki and Mr. T. Kikuchi



## Award Ceremony for JSCES Prizes

A fter the meeting, JSCES prizes were offered to senior and young researchers and practitioners (*Figure 3*). This year's recipients are Dr. Motoi Okuda (The JSCES Achievement Award), Prof. Daigoro Isobe (Kawai Medal), Dr. Yuuichiro Yoshida (Shoji Medal), Dr. Keizo Ishii and Mr. Makoto Tsukino (Technology Prize), and Dr. Takaya Kobayashi (Technology Prize).

## Prof. Tadahiko Kawai's achievements and contributions

**Prof. Tadahiko Kawai** passed away in Tokyo on October 31, 2014 at age 88 (*Figure 4, Figure 5*).

Prof. Kawai graduated from the Department of Naval Architectural Engineering in 1952 and continued to the school of engineering at the University of Tokyo, Japan. He received Ph.D. degrees from Lehigh University, USA in 1957 and from the University of Tokyo in 1962. Prior to joining the University of Tokyo in 1963, he worked for National Aerospace Laboratory of Japan for 5 years. He was one of the pioneers of finite element methods in Japan and contributed enormously to the societies of computational solid mechanics in the world.

Prof. Kawai was well known for his Kawai model, the RBSM,

which created and experted the field of discrete limit analysis. He developed the model in the 1970's, realizing the strong needs of the numerical analyses on limit status of structures and progressive damage behavior. He was recently working on the generalization of the energy principles; the new outcomes in his study will be published from the JSCES this year.

One of the great achievements of his continuous schooling of finite element methods was the success of WCCM-III held in 1994, Japan, in which he made effort to attract researchers in the field of computational mechanics all over the world. After WCCM-III, Prof. Kawai founded the JSCES and was inaugurated as the first president. He also served as a vice-president of the IACM. Prof. Kawai has spent lots of time for discussions especially with young researchers with enthusiasm since the dawn of computational mechanics. At the same time, he contributed greatly to their education, hoping for their continued growth and success. Taking over with his intention, the JSCES established the Kawai Medal to commend young researchers for their outstanding achievements in the field of computational engineering and science.

In this way, his long-term great contribution to our societies for computational mechanics and applied mechanics should be long remembered. The death of Prof. Kawai is a profound regret for our societies in the fields. We express our deep and sincere condolences to his family.

*Figure 5:* Group shot at Prof. J.T. Oden's Honda Award commemoration party held in 2013

Paper awards associated with the Transaction of the JSCES (see, https://www.jstage.jst.go.jp/browse/jsces) were also given to the following researchers: Prof. Shigenobu Okazawa, Mr. Koji Nishiguchi and Prof. Satoyuki Tanaka (Outstanding Paper Award), Mr. Norimasa Yamasaki (Outstanding Paper Award), Prof. Mao Kurumatani (Young Researcher Paper Award), Mr. Takahiro Kikuchi (Young Researcher Paper Award) (*Figure 3*).

The JSCES Grand Prize, the highest award in JSCES, was given to Prof. René de Borst of University of Glasgow at the 20th JSCES's Annual Conference on Computational Engineering and Science, which was held on June 8-10, 2015, at Tsukuba International Congress Center, Ibaraki, Japan.



Figure 4: Group shot at Venice in 1990







Figure 1: Shinobu Yoshimura, President



**Figure 2:** Takayuki Aoki, Vice President



Figures 3: Shinji Nishiwaki, Vice President



Figures 4: Hiroshi Okada, Secretary General

## JAPAN ASSOCIATION FOR COMPUTATIONAL MECHANICS

The JACM is a union of researchers and engineers working in the field of computational mechanics mainly in Japan. The number of individual members is about 300. From March, 2015, the following three societies, The Japan Fluid Power System Society, The Japan Society of Naval Architects and Ocean Engineering, and Meteorological Society of Japan, have newly joined in JACM, and the JACM is now collaborating with totally 29 computational mechanics related societies in Japan. See in more detail our web page (http://www.sim.gsic.titech.ac.jp/jacm/index-e.html).

In March 2015, JACM formed the new General Council members and elected its executive council members for 2015-2017 as follows. They continue to serve following their three-year appointment of 2012-2014.

## President: Professor Shinobu Yoshimura,

The University of Tokyo. yoshi@sys.t.u-tokyo.ac.jp, http://save.sys.t.u-tokyo.ac.jp/prof/index.html Vice Presidents: Professor Takayuki Aoki, Tokyo Institute of Technology. taoki@gsic.titech.ac.jp, http://www.sim.gsic.titech.ac.jp/English/Member/taoki.html and Professor Shinji Nishiwaki,

*Kyoto University.* shinji@prec.kyoto-u.ac.jp, http://www.osdel.me.kyoto-u.ac.jp/english/members/index.html **Secretary General:** *Professor Hiroshi Okada*, *Tokyo University of Science.* hokada@rs.noda.tus.ac.jp, http://www.rs.noda.sut.ac.jp/me/laboratories/okada\_laboratory.html

JACM participated the **Fourth Computational Mechanics Symposium** organized by the **Science Council of Japan (SCJ)**, on **December 1, 2014**. The function of SCJ is defined as "The Science Council of Japan was established in 1949 as a "special organization" under the justification of the Prime Minstar, operating independently of the government for the purpose of promoting and enhancing the field of science, and having science reflected in and permeated in administration, industries and people's lives. It represents Japan's scientists both domestically and internationally ..." (http://www.scj.go.jp/en/scj/index.html). The SCJ Computational Mechanics Symposium has become an annual event and is an evidence of how Japanese science and engineering community finds computational mechanics to be a very important area.

In the fourth symposium, eight excellent young researchers representing the participating computational mechanics related societies presented their latest research outcomes.

The other participating societies are: The Japan Society of Mechanical Engineers (JSME), The Japan Society for Industrial and Applied Mathematics (JSIAM), The Japan Society for Computational Engineering and Science (JSCES), The Japan Society for Simulation Technology (JSST), The Visualization Society of Japan (VSJ), CAE Konwakai and Japan Society for Computational Methods in Engineering (JASCOME). From JACM, Professor Satoshi Ii of Osaka University, who is the recipient of 2014 JACM Young Investigator Award, presented the latest research outcomes of his novel fixed-grid finite difference scheme for fluid-structure interaction analyses with biomechanics applications.

The symposium started with the opening remark by Professor Genki Yagawa (SCJ Member, Former President of IACM). Then, presentations by the young researchers followed:

- **Professor Takaharu Yaguchi** (JSIAM, Kobe University) on Hamilton equations
- **Professor Toru Takahashi** (JASCOME, Nagoya University) on acceleration of BEM computations
- Professor Tomohiro Takaki (CAE Konwakai, Kyoto Institute of Technology) on large scale phase-field simulation on metallographic structures
- Professor Mao Kurumatani (JSCES, Ibaraki University) on an isotropic damage model based on fracture mechanics for concrete
- Tetsuya Matsuda (JSME, University of Tsukuba) on nonlinear multiscale analyses for fiber reinforced composite materials,
- Professor Satoshi Ii (JACM, Osaka University) on fixed-grid finite difference scheme for fluid-structure interaction analyses
- Dr. Naoya Tsuruta (JSST, University of Tsukuba) on ORIGAMI folding design
- Dr. Masaki Yoshida (VSJ, Japan Agency for Marine–Earth Science and Technology) on numerical simulation of 3-D mantle convection.

After the scientific presentations and discussions, the symposium ended by the closing remark of Professor Ichiro Hagiwara (SCJ Member, Meiji University).

*Figure 5: Symposium Venue: Auditorium, Science Council of Japan* 



## Figures 6:

Organizers and speakers of computational mechanics symposium (From left: Prof. I. Hagiwara, Prof. G. Yagawa, Dr. N. Tsuruta (JSST), Prof. M. Kurumatani (JSCES), Prof. S. Ii (JACM), Prof. T. Matsuda (JSME), Prof. T. Takaki (CAE Konwakai), Prof. S. Yoshimura (President, JACM)



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## **PANACM 2015**

The First Pan-American Congress on Computational Mechanics, PANACM 2015 and the XI Argentine Congress on Computational Mechanics, MECOM 2015, took place in Buenos Aires, Argentine, April 27 - 29, 2015.

PANACM 2015 is the first conference organized under the auspices of the International Association for Computational Mechanics (IACM) to promote the Computational Mechanics in the Americas as a one region. During the WCCM 2012 in Sao Paulo, Brazil, the national associations of the Americas decided the periodic organization of a Pan-American congress, whose first edition took place in Buenos Aires in 2015.

This Congress was organized in conjunction with the XI Argentine Congress on Computational Mechanics, MECOM 2015, a traditional and very well known congress in the Argentinean science community, and attracted around 600 participants, coming from all over the world. All together some 540 lectures, organized in 45 Mini-Symposia, have been presented, including 8 Plenary lectures, 12 Semi-Plenary lectures and 43 Keynote Lecturers, which reflect the current state of the research and advances in engineering practice in the Computational Mechanics science.

Delegates from 38 countries participate at PANACM 2015, the main participation corresponding to: Argentina 133, Brazil 81, United States 78, Chile 29, France 28, Japan 27, Spain 25, Germany 22, Italy 11, and Poland 11.

The International Centre for Numerical Methods in Engineering (CIMNE) organized this Conference jointly with the Asociación Argentina de Mecánica Computacional (AMCA).

Submitted full papers have been published in an e-book, available on the website: http://congress.cimne.com/panacm2015/frontal/doc/EbookPANACM2015.pdf.

## International AMCA Award 2014

During PANACM the **AMCA Award 2014** to the International Scientific Career was delivered to **Prof. Tom J. R. Hughes**, from the University of Texas at Austin, USA.

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The AMCA Awards are delivered, every two years, as recognition of the scientific trajectory in the field of computational mechanics and are granted in three categories: Young Researchers; Scientific, Professional and Teaching Trajectory; and International Scientific Trajectory. The last one have been instituted to recognize not only the scientific trajectory in the field of computational mechanics but also the interaction with research centres of Argentina, or with argentine researchers.

## Figure 1:

Prof. Victor Calo, an argentinean former Ph.D student of Prof. Hughes, given the AMCA prize to the awarded, during the appreciation dinner of the PANACM Conference

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Plenary Speakers of PANACM 2015 were: K.-J. Bathe, L. Caffarelli, Ch. Farhat,
T. J. R. Hughes, E. Oñate, O. Pironneau, E. Ramm and P. Wriggers.
Semi-Plenary Speakers were: G. Buscaglia, A. Cardona, A. Cuitiño, L. Demkowicz,
E. Dvorkin, I. Gamba, A. Huerta, A. Loula, X. Oliver, R. Rodriguez, M. Storti and F. Valentin.

PANACM 2015 was supported by the following IACM American Affiliated Associations:

Argentine Association for Computational Mechanics (AMCA), Mexican Association for Numerical Modeling and Engineering (AMMNI) Brazilian Association for Computational Methods in Engineering (ABMEC) Colombian Association for Numerical Methods in Engineering and Applied Sciences (ACMENICA)

Chilean Association for Computational Mechanics (SCMC) U.S. Association for Computational Mechanics (USACM) Venezuelan Society for Numerical Methods in Engineering (SVMNI)

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*Figure 3:* Lecture of Prof. Charbel Farhat

Figure 4: Dr. Lino Barañao, Minister of Science, Technology and Productive Innovation of Argentina, speaking at the opening ceremony

*Figure 5:* One of the PANACM Coffee Breaks at the Hilton Hotel

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## CILAMCE 2015

## he CILAMCE 2015 – XXXVI Ibero-Latin American Congress on

**Computational Methods in Engineering** will take place in Rio de Janeiro, Brazil, from **22 to 25 November 2015**. CILAMCE is an annual conference – promoted by the Brazilian Association of Computational Methods in Engineering (ABMEC) – intended as an international forum for communicating recent developments of numerical methods in several engineering areas. Since 1977, when it was founded by the emerging Brazilian community of computational mechanics under the leadership of the late Prof. Agustín Ferrante, CILAMCE has become the main opportunity for engineers, students, researchers and other professionals mainly from Brazil and Latin-America to discuss and explore the state of the art of computational methods.

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CILAMCE is a multidisciplinary event: scientists and engineers from all over the world are encouraged to attend the conference. The technical program will include six invited plenary speakers and a large number of mini-symposia with contributed papers.

As it already has become a tradition, there will be a special competition – the Agustín Ferrante Award – to acknowledge undergraduate students who show potential for outstanding scientific achievements.

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XXXV·Iberian·Latin·American·Congress·on· Computational·Methods·in·Engineering· CILAMCE·2014¶

The XXXV Iberian Latin American Congress on Computational Methods in Engineering (CILAMCE) was held in Fortaleza, in November 23rd to 26th, 2014. Fortaleza is the state capital of Ceará, located in Northeastern Brazil. It is the 5th largest city in Brazil and a major and an enchanting tourist destination.

This CILAMCE edition was hosted by the Graduate Program in Structures and Civil Construction of the Federal University of Ceará (PEC/UFC).

CILAMCE, promoted by the Brazilian Association of Computational Methods in Engineering (ABMEC), provides an enriching forum for engineers, students, researchers and other professionals active in the field of numerical methods not only from Brazil, but from worldwide. In its 2014 edition, CILAMCE had 450 participants, including engineers, professors, and graduate and undergraduate students. The participants came from 9 different countries, such as United Kindom, Portugal, Germany and Peru, in addition to a great number of Brazilians.

The technical program included plenary speakers and mini-symposia sessions on different topics related to computational methods in engineering. In this edition, over 370 works were presented in different 26 mini-symposia.

Also, during CILAMCE 2014, the re-elected ABMEC Directing Board for the next two years was presented: Prof. Gray Farias Moita (president) from Centro Federal

This year's edition of CILAMCE has a special flavor, since the hosting Graduate Program in Civil Engineering at PUC-Rio is celebrating its 50th anniversary. It is also coincidentally the 450th anniversary of the City of Rio de Janeiro. This is a motivation to celebrate the CILAMCE 2015 not only as an academic event of excelling characteristics but also as an occasion to gather a large number of our Graduate Program's more than 1000 former M.Sc. and Ph.D. students spread all over the world.

The venue is a comfortable and well-equipped hotel situated on the celebrated Copacabana beach. Rio de Janeiro is at a one-flight distance from most large cities in the world. Although accessing the Rio Othon Palace Hotel by car, bus or subway is a simple matter, participants may want to examine logistics recommendations and offers.

The reasons to join the conference, contribute to its success and enjoy this lovely city are numerous. We are looking forward to sharing this unique event with you next November in Rio de Janeiro!

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Figure 1: (left) Opening speech, Prof. Evandro Parente, Congress Chairman Figure 2: (middle) Plenary Lecture, Prof. Peter Wriggers Figure 3: (right) Plenary Lecture, Prof. Sergio Idelsohn

de Educação Tecnológica de Minas Gerais, Prof. Paulo Roberto Maciel Lyra (vice-president), Prof. Sylvia Regina Mesquita de Almeida (1st secretary), Prof. Roberto Dalledone Machado (2nd secretary) and Prof. José Ricardo Queiroz Franco (treasurer).

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**Figure 5:** (below) Agustin Ferrante Award for best undergraduate paper Figure 4: (left) Opening Ceremony

*Figure 6:* (below left) Congress Banquet

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## 3rd German-Japanese Workshop on **Computational Mechanics**

he 3rd German-Japanese Workshop on Computational Mechanics, a joint initiative of the German Association for Computational Mechanics (GACM) and the Japanese Society for Computational Engineering and Science (JSCES), was held in Munich (Germany) on March 30th and 31st, 2015, thus continuing the long-standing tradition of this workshop series with previous editions having been held in Yokohama (Japan) and Hannover (Germany).

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real-world engineering applications.

both senior faculty members and young investigators, have spent two days discussing the latest developments in the broad field of computational mechanics and intensifying the scientific relationship and the friendship between German and Japanese researchers. The invited talks covered an enormous width of topics from cutting-edge computational engineering and science research, including computational solid and fluid dynamics, multi-scale and coupled multi-field problems, reduced-order modeling, uncertainty quantification, biomedical engineering and many more, with their focus being on the entire spectrum of modeling and simulation activities ranging from fundamental mechanical modeling, development of numerical

More than 30 participants from the two countries, including

**Alexander Popp** Wolfgang A. Wall

On behalf of the organizing committee D. Isobe (University of Tsukuba) K. Kashiyama (Chuo University) A. Popp (Technical Univ. of Munich) K. Terada (Tohoku University) W.A. Wall (Technical Univ. of Munich) P. Wriggers (Leibniz Univ. of Hannover)

Four keynote lectures have been delivered by Marie Oshima (The University of Tokyo), Sigrid Leyendecker (University of Erlangen), Toshio Nagashima (Sophia

University) and Michael Kaliske (Technical University of Dresden).

methods and computational algorithms to high-performane computing and innovative

With the aim of the workshop being not only to strengthen the scientific relationships between Germany and Japan, but also to give the participants a possibility of personal encounter and exchange in a cordial atmosphere, a social evening and dinner in a typical Bavarian restaurant was also on the list of activities. After two interesting days with inspiring talks and ideas, fruitful scientific discussions, the reunion with old friends and the building of new friendship, GACM and JSCES are determined to continue the success story of this workshop series.

> Figure 1: German-Japanese Workshop Participants (Photo: Christian Roth)

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## *10th International Workshop on* Variational Multiscale and Stabilized Finite Elements (VMS2015)

The 10th International Workshop on Variational Multiscale and Stabilized Finite Elements (VMS2015), organized under the auspices of GACM by Volker Gravemeier and Wolfgang A. Wall, was held on **February 25 to 27, 2015** at the Institute for Computational Mechanics at the Technische Universiät München. About 30 researchers participated in VMS2015 and presented both novel theoretical developments as well as applications. Along with the tradition of the VMS workshops, the majority of presentations covered various problems of fluid mechanics. However, other interesting and challenging applications ranging from transient solid dynamics to plasma physics were also addressed.

Figure 2: Some VMS Workshop Participants (Photo: Christian Roth)

2nd International Workshop on Latest Advances in Cardiac Modeling (LACM 2015)

On March 12 -13 2015 the 2nd International Workshop on Latest Advances in Cardiac Modeling (LACM 2015) was held at the German Heart Center in Munich under the auspices of GACM. The goal of LACM 2015 was to bring together top level researchers focused on methodological aspects of mathematical and computational modeling of the heart. The workshop had two plenary talks, namely Jean-Frédéric Gerbeau from INRIA Paris-Rocquencourt and Sebastian Kozerke from ETH Zürich, plus more than 30 contributed presentations. Topics included: Novel mathematical

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models for cardiac tissue (e.g. electrophysiology, active/passive mechanics), and their analysis; Numerical algorithms for the solution of partial differential equations used for modeling the cardiac behavior; New data acquisition techniques relevant for modeling (in particular MRI); Validation of models and simulation tools with real data; Biophysical personalization of models through data assimilation; Computational simulations addressing relevant clinical problems.

The organizers, Cristobal Bertoglio, Isabel Deisenhofer, Markus Schwaiger and Wolfgang A. Wall, warmly thank all participants and together with them look forward to a next version of the workshop!

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The new **GACM Report**, issue No. 9, just appeared. This issue is dedicated to contributions from industry and hopes to further foster exchange between academia and industry. An online version of the report can be found on the webpage of GACM at **www.gacm.de**.

Figure 3: Previous issues of GACM report

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## AIMETA

Associazione Italiana di Meccanica Teorica e Applicata

## **GIMC Upcoming Conferences**

The Italian Group of Computational Mechanics GIMC would like to inform you about their upcoming conferences:

## AIMETA

XXII Congress of the Italian Association of Theoretical and Applied Mechanics 14-17 September 2015, University of Genova, Italy

The Congress of the Italian Association of Theoretical and Applied Mechanics – AIMETA, for almost fifty years has been an opportunity for discussion between researchers in the fields of General Mechanics, Mechanics of Fluids, Solids and Structures, Machine and Construction of Machines.

Within the Conference, the Italian Group of Computational Mechanics – GIMC – organizes a minisymposium with the aim to provide a forum for discussing advantages, drawbacks, new possibilities and applications of the forefront of Computational Mechanics. The minisymposium seeks at gathering researchers and scholars working on conception, development, mathematical analysis, and validation of advanced numerical methods and modern computational techniques. The MS also welcomes researchers devoted to the development of innovative applications of more classical computational techniques.

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The conference topics include fundamental research, applications and computational studies devoted to the progress of extended and specialized discretization methods such as, but not limited to: Partition of Unity methods (Meshfree, XFEM/GFEM); Patch Methods; Fictitious Domain Methods; Strong Discontinuity Approaches (SDA); Local/Global Non-Intrusive Coupling; Finite

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Cell Methods; Multiscale Discretization; Special techniques for static and evolving interfaces; Crossover approaches, such as integration of PUFEM with isogeometric method.

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## KSCM

h the CCM XII c c World Congress on Computational Mechanics

24-29 July **2016** 

Seoul, Korea

900M2

## 

Asia-Pacific Congress on Computational Mechanics

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## conference diary planner

6 - 10 July 2015	ESMC 2015: 9th European Solid Mechanics Conference		
	Venue: Ljubljana, Slovenia Co	ontact: http://www.icoev.org/	
13 - 15 July 2015	FEM/MESHLESS 2015 : Finite Elemen	ts and Meshless Methods for Science and Engineering	
	Venue: Porto, Portugal Co	ontact: https://sites.google.com/site/femmeshless2015/	
20 - 23 July 2015	6th GACM Colloquium and 3rd ECCO	MAS Young Investigator Conference	
	Venue: Aachen, Germany Co	ontact: http://www.gacm.de/index.php?id=21	
26 - 30 July 2015	USNCCM13: U.S. National Congress of	on Computational Mechanics	
	<i>Venue:</i> San Diego, CA Co	ontact: http://13.usnccm.org/	
1 - 3 Sept 2015	COMPLAS XIII: International Confere	nce on Computational Plasticity	
	<i>Venue:</i> Barcelona, Spain <i>C</i> o	ontact: complas@cimne.upc.edu	
8 - 11 Sept 2015	CMM: 21st International Conference of	on Computer Methods in Mechanics	
	Venue: Gdańsk, Poland Co	ontact: http://www.pcm-cmm-2015.pg.gda.pl/	
9 - 11 Sept 2015	X–DMS 2015: eXtended Discretization Methods		
	Venue: Ferrara, Italy Co	ontact: http://x-dms2015.sciencesconf.org/	
14 - 16 Sept 2015	ICCB'2015: Sixth International Confer	ence on Computational Bioengineering	
	Venue: Barcelona, Spain Co	ontact: iccb2015@cimne.upc.edu	
21 - 23 Sept 2015	IMACA 2015: Integrated Modeling and	Analysis in Applied Control and Automation	
	Venue: Bergeggi, Italy Co	ontact: sjunco@fceia.unr.edu.ar	
21 - 23 Sept 2015	PARTICLES 2015: IV International Co	nference on Particle-based Methods	
	Venue: Montenegro Co	ontact: http://www3.imperial.ac.uk/aeronautics	
23 - 29 Sept 2015	ICNAAM 2015: Numerical Fluids 2015		
	Venue: Rhodes, Greece Co	ontact: http://www.icnaam.org/nafluids	
28 - 30 Sept 2015	FDM 2015: Fracture and Damage Mec	hanics	
	Venue: Barcelona, Spain Co	ontact: particle-basedmethods@cimne.upc.edu	
29 Sept - 2 Oct 2015	ICCSM 2015: 8th International Congre	ess of the Croatian Society of Mechanics	
	Venue: Opatija, Croatia Co	ontact: http://www.ceacm.org/	
12 - 14 Oct 2015	IWACOM: International Workshops or	Advances in Computational Mechanics III	
	Venue: Tokyo, Japan Co	ontact: http://www.jsces.org/IWACOM/	
19 - 21 Oct 2015	STRUCTURAL MEMBRANES 2015: VI	I Int. Conf. on Textile Composites & Inflatable Structures	
	Venue: Barcelona, Spain Co	ontact: membranes@cimne.upc.edu	
4 - 6 Nov 2015	3rd Workshop Reduced Basis, POD o	r PGD-Based Model Reduction Techniques	
	Venue: Cachan, France Co	ontact: http://www.iacm.info	
22 - 25 Nov 2015	CILAMCE 2015: Ibero-Latin American	Congress on Computational Methods in Engineering	
	<i>Venue:</i> Rio de Janeiro, Brazil Co	ontact: http://www.cilamce.com.br/	
5 - 10 June 2016	ECCOMAS Congress 2016		
	Venue: Crete Island, Greece Co	ontact: http://eccomas2016.org/	
11 - 14 July 2016	ICCMS2016 : VI Int. Congress on Com	putational Mechanics and Simulation	
	Venue: Bologna, Italy Co	ontact: http://conference.mercatura.pt/mechcomp2016/	
24 - 29 July 2016	APCOM 2016: 6th Asia Pacific Congress on Computational Mechanics		
	Venue: Seoul, Korea Co	ontact: http://apacm-association.org	
24 - 29 July 2016	WCCM XII: World Congress on Comp	utational Mechanics	
	Venue: Seoul, Korea Co	ontact: http://www.wccm-apcom2016.org/	
21 - 26 Aug 2016	24th International Congress of Theore	etical and Applied Mechanics	
	Venue: Montreal, Canada Co	ontact: http://www.ictam2016.org/	