

**Moving Particle Semi-implicit
(MPS) Method - Application
to Free Surface Flow**

S. Koshizuka

**Advanced Computational Methods
to Understand & Mitigate
Extreme Events**

M. Hillman, J. S. Chen & M. J. Roth

**Computational Mechanics in
South Africa (and Beyond)**

B. D. Reddy

Data-Driven Computing

M. Ortiz & T. Kirchdoerfer

**A Finite Element Primer
for Beginners: The Basics**

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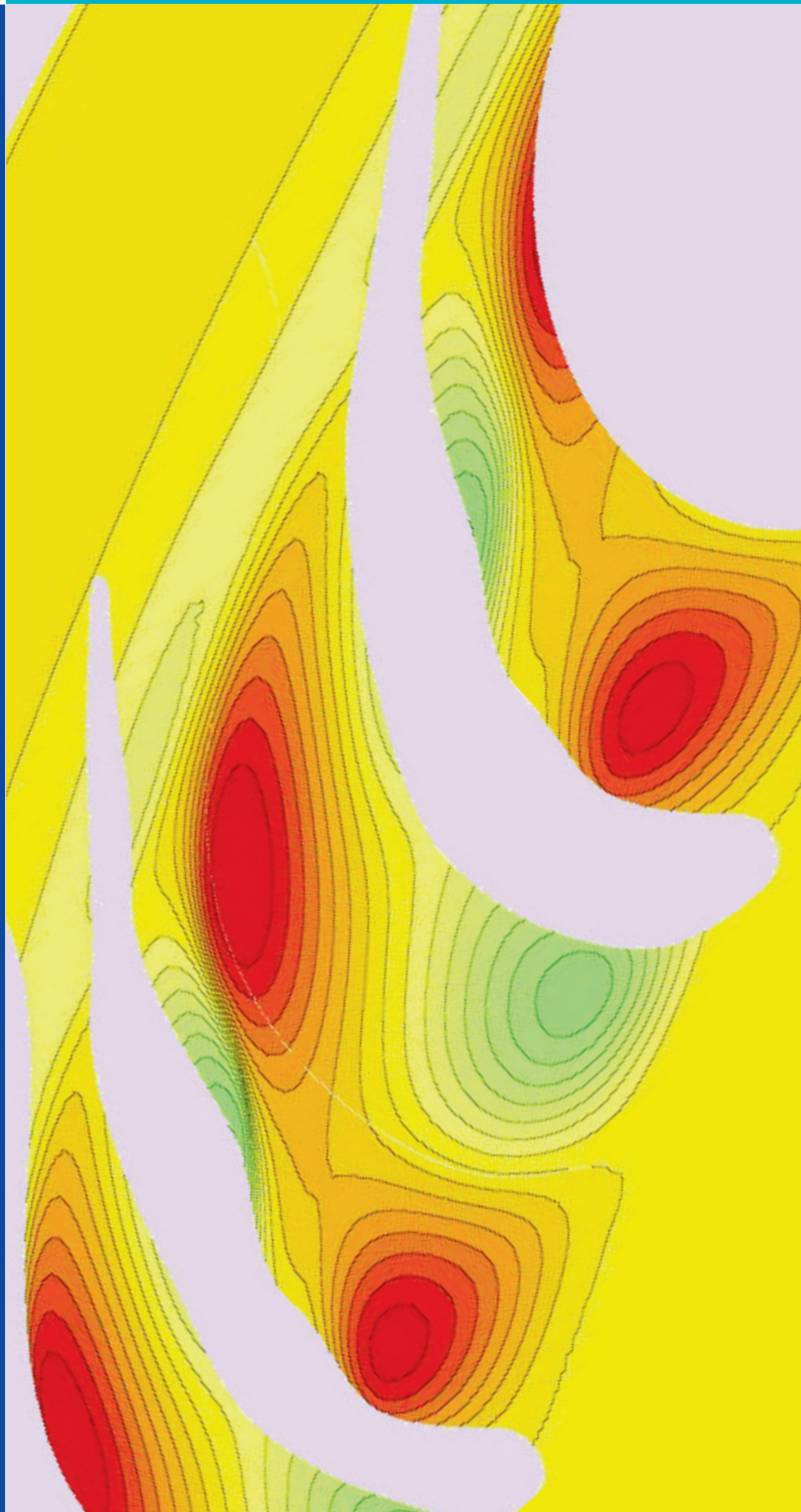
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- 2 **Moving Particle Semi-implicit (MPS) Method - Application to Free Surface Flow**
S. Koshizuka
- 6 **Computational Mechanics in South Africa (and Beyond)**
B. D. Reddy
- 10 **Data-Driven Computing**
M. Ortiz & T. Kirchdoerfer
- 12 **Advanced Computational Methods to Understand & Mitigate Extreme Events**
M. Hillman, J. S. Chen & M. J. Roth
- 17 **Book Report - A Finite Element Primer for Beginners: The Basics, by T. I. Zohdi**
Review by D. Givoli
- 20 **UKACM** United Kingdom
- 22 **CSMA** France
- 24 **JSCES** Japan
- 26 **JACM** Japan
- 28 **AMCA** Argentina
- 30 **GACM** Germany
- 32 **USACM** United States of America
- 34 **Conference Diary Planner**

contents

editorial

Mesh-free methods (also known as meshless methods) have been a promising procedure during the last few decades for the numerical solution of many problems in engineering and applied sciences. The essence of mesh-free methods is the approximation in space of the unknown field in terms of the information in a set (cloud) of arbitrarily distributed points within the analysis domain. The existing mesh-free methods differ on the way the approximation is performed, via different space interpolation procedures, and also in how the derivatives of the unknown field are computed over the cloud of points. In essence a truly mesh-free method does not require a mesh for the integration of the governing equations in mechanics over the analysis domain and use point collocation for this purpose. Among the many meshless methods we mention the generalized finite differences method, the smooth particle hydrodynamics (SPH) method, the diffusive element method, the element-free Galerkin (EFG) method, the reproducing kernel particle method (RKPM), the natural element method (NEM), the local radial point interpolation method, the moving particle semi-implicit (MPS) method and the finite point method (FPM), just to name a few.

Differently from the “truly” meshless methods, other numerical techniques use a cloud of points for the purposes of interpolating the unknown field only, but integrate the governing equations over a background mesh that discretizes the analysis domain. This category of numerical procedures can be classed under the wider range of particle-based methods. Some examples are the particle-in-cell (PIC) method, and its variant the material point method (MPM), and the particle finite element method (PFEM), among others.

In most meshless and mesh-based methods mentioned above the points in the cloud are treated as material points characterized by the density of the underlying domain, an exception to this being the SPH and MPM methods that assign a mass to each point in the cloud. Hence, these methods should not be confused with the wide class of methods that use discrete particles for studying the mechanics of a physical system containing a finite collection of small or large objects. The most popular method of this kind is the discrete element method (DEM). It is interesting that this class of

particle-based numerical methods have also promising features for solving continuum mechanics problems.

The number of scientific publications and international conferences and workshops on meshless and particle-based methods has substantially increased in recent years. Many of these activities are supported by the IACM and its regional organizations worldwide. This has been due to the growing interest of industry for these numerical procedures, ranging from the classical manufacturing industries to the new additive manufacturing technology, and also to the civil engineering, mining, oil and gas, pharmaceutical, bio-medical and food processing industries, just to name a few.

This issue of Expressions includes two articles describing the main features and recent advances of the MPS and the RKPM meshless techniques applied to fluid dynamics and extreme events, respectively. Certainly, the progress of meshless procedures is tightly connected to that of the fast generation of large sets of point clouds, error estimation, point adaptivity and visualization of large sets of results using distributed computing techniques, among others. Looking to the progress in these fields I anticipate that we are going to hear more in the near future of the meshless analysis techniques.

By the time you read these lines most probably the 12th World Congress on Computational Mechanics (WCCM XII) and the 6th Asia-Pacific Congress on Computational Mechanics (APCOM VI) will have taken place in Seoul, Korea, on 24 – 29 July 2016. The joint event has attracted over 2000 participants from all over the world. I express my congratulation to the organizers for this success.

The WCCM XII and XIV will be respectively held in New York and Paris on 2018 and 2020. These look like good busy times ahead for the computational mechanics community. Please check the IACM web page for the details of these and many other smaller thematic scientific events to be held worldwide in the next coming years.

Eugenio Oñate
Editor of IACM Expressions

Moving Particle Semi-implicit (MPS) Method

- Application to Free Surface Flow

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“ ... MPS ...
is a powerful
tool to analyze
fluid flow with
complex motion
of free surface.”

The Moving Particle Semi-implicit (MPS) method has been developed and applied to fluid flow with large deformation of free surfaces. The distinct difference between MPS and Smoothed Particle Hydrodynamics (SPH) is discretization formulation for differentiations. Recent applications of the MPS method to free surface flow are provided: oil flow and torque evaluation in a crankcase, deaeration from the free surface in a mixing tank, and tsunami run-up on the nuclear power plant site and subsequent flooding in a building.

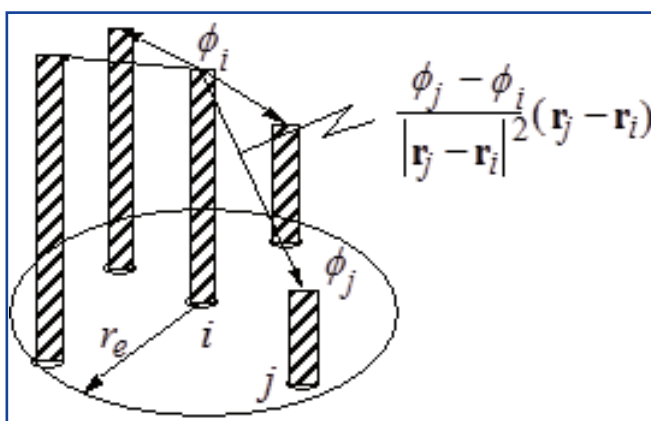
Introduction

Moving Particle Semi-implicit (MPS) method is one of the particle methods which can be applied to fluid flow [1]. Since the mesh is not necessary, large deformation of free surfaces can be analyzed without mesh distortion. The governing equations are represented by Lagrangian description and it is not necessary to discretize the convection terms. This keeps the free surfaces clear without numerical diffusion which is derived from the discretization process of the convection terms. Thus, the particle methods are expected to be applied to fluid flow accompanied by complex motion of the free surfaces [2]. The present article provides a brief introduction to the MPS method and recent application examples to fluid flow analysis with the free surfaces.

MPS method

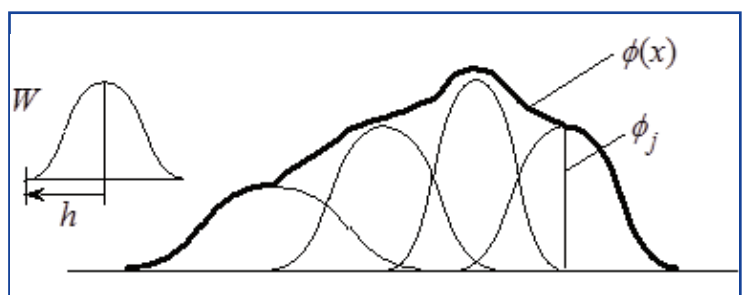
A semi-implicit algorithm was proposed for incompressible flow with the free surfaces in the MPS method [1]. This algorithm was adopted in another particle method, Smoothed Particle Hydrodynamics (SPH), and called Incompressible SPH (ISPH). There is a distinct difference between MPS and SPH. In MPS, discretization of a differentiation is performed as a weighted difference as shown in *Figure 1 (a)*. A difference can be obtained between two values at two particles. Weighted average of the differences among the neighboring particles within the influential radius is obtained at the particle position. In SPH, a global distribution of the variable is first assumed as superposition of the kernel then discretization is performed based on this variable distribution as shown in *Figure 1 (b)*. Therefore, the derivative of the kernel appears in the discretized formulations. The explicit algorithm using pseudo-compressible governing equations is now used in both SPH and MPS [3] as well as the semi-implicit algorithm.

In MPS, the differential operators are discretized without assuming the global distribution of the variables. Thus, different weight functions and different influential radii can be employed for different operators; for example, the influential radius for the Laplacian operator is usually larger than that for the gradient



(a) MPS

Figure 1:
Comparison between MPS and SPH



(b) SPH



Figure 2:
Oil circulation in a crankcase (1,750rpm)

operator from the viewpoint of numerical accuracy and stability. In SPH, since the global distribution of the variable is assumed, all the kernels and the influential radii of various differential operators should be the same. Therefore, MPS is more flexible than SPH, in particular, for modeling various physics. This flexibility is important for a wide range of applications.

Higher order schemes of MPS was studied on the basis of the least square method [4]. Convergence of the schemes was verified. The compact scheme, a smaller number of particles is necessary for a higher order scheme, was also included in the generalized formulation. From this study, the conventional MPS method is regarded as a low order scheme with simplified formulation.

Fluid flow analysis with the free surfaces

Simulations and experiments of oil flow in a simplified crankcase were carried out. *Figure 2* shows the result of 1,750 rpm. We can see oil circulation around the rotating crank. Oil splashing which is observed in the experiment is approximately reproduced in the simulation.

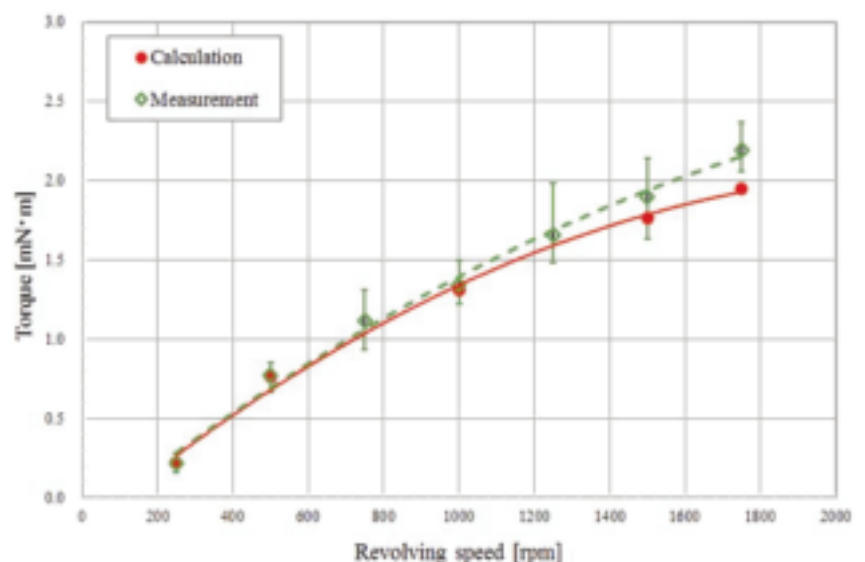
Figure 3 shows comparison between the measured torques in the experiments and the evaluated ones in the simulations. Good agreement is obtained when the rotating speed is low. The deviation is larger when the rotating speed is higher. This is due to the effect of small bubbles involved in the oil. When the rotating speed is higher, more bubbles are generated and contained in the oil. This increases the oil surface level, which enhances the torque.

The uncertainty of the spatial resolution was evaluated at 1,750 rpm using Grid Convergence Index (GCI) [6]. Three cases were calculated using 6689, 58858 and 477543 oil particles. It was found that

the convergence had the order of 2.10 and the converged torque value was 2.17 mN·m. GCI was 3.04%.

In the chemicals process, small bubbles are often generated as a product of chemical reaction in a mixing tank. Deaeration from the free surface was analyzed using the MPS method [7]. The mole of gas in the bubbles was represented by a variable of each liquid particle. The bubble motion was basically traced as the Lagrangian description of the liquid particles. The buoyancy effect was modelled as the transport of the mole from the lower particles to the upper particles. The deaeration on the free surface was modelled as the decrease of the mole on the free surface with a time constant.

Figure 3:
Comparison of torque: calculation and experiment



It was assumed that the bubbles were initially located in the bottom region of the mixing tank. Two types of the rotating blades were used: paddle and anchor. The calculation results using the paddle and anchor blades are depicted in

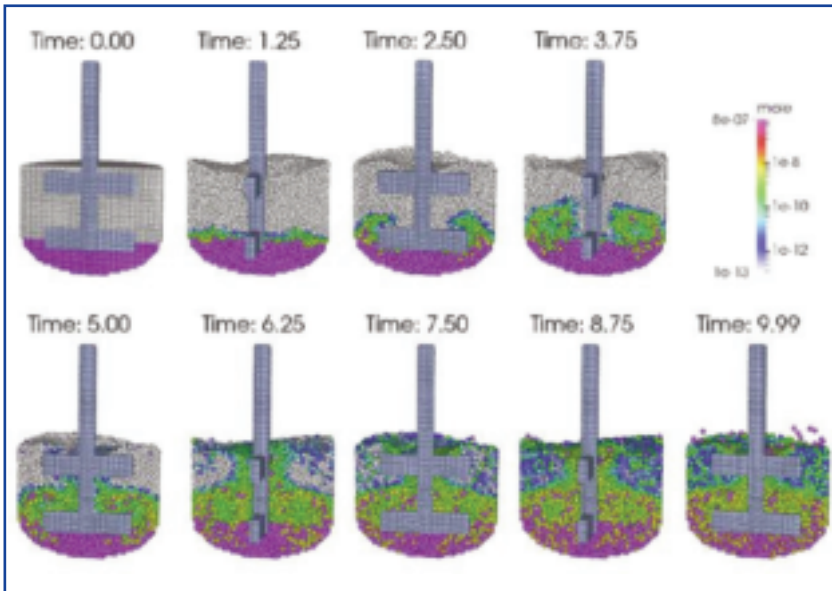


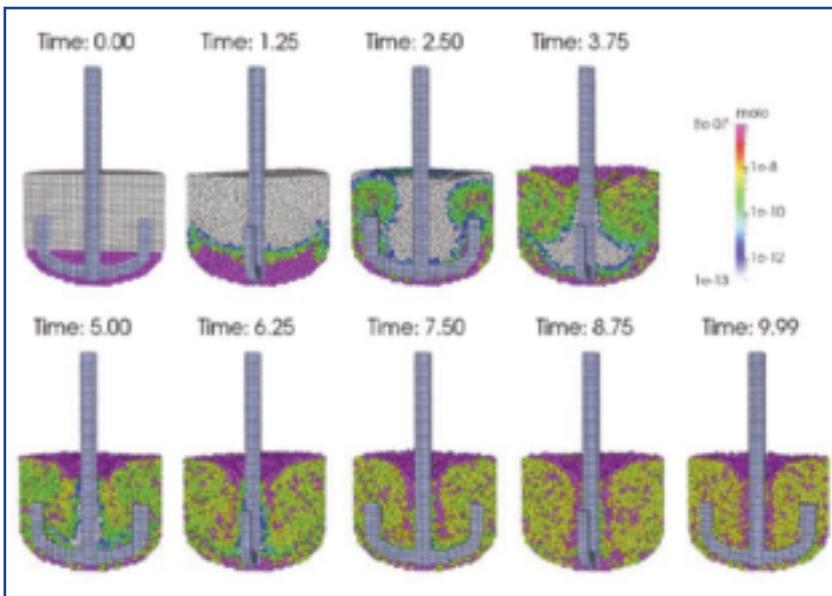
Figure 4:
Deaeration from free surface in mixing tank with paddle blades

Figures 4 and 5, respectively. When the paddle blades are used, two circulation flows appear in the tank and the bubbles stay in the lower region for a long time. When the anchor blades are used, a vertical circulation makes the upper flow and deaeration is quicker.

The MPS method was applied to large-scale tsunami run-up simulation using a dynamic domain decomposition technique for parallel computing. Figure 6 illustrates the computer graphics image of the simulation result when a large tsunami comes to the nuclear power plant site. The wave shape was assumed as that of the Great East Japan Earthquake in 2011. We can see the inundation area in Figure 6. In this simulation, 250,000,000 particles were used with the size of 1m.

Figure 5:

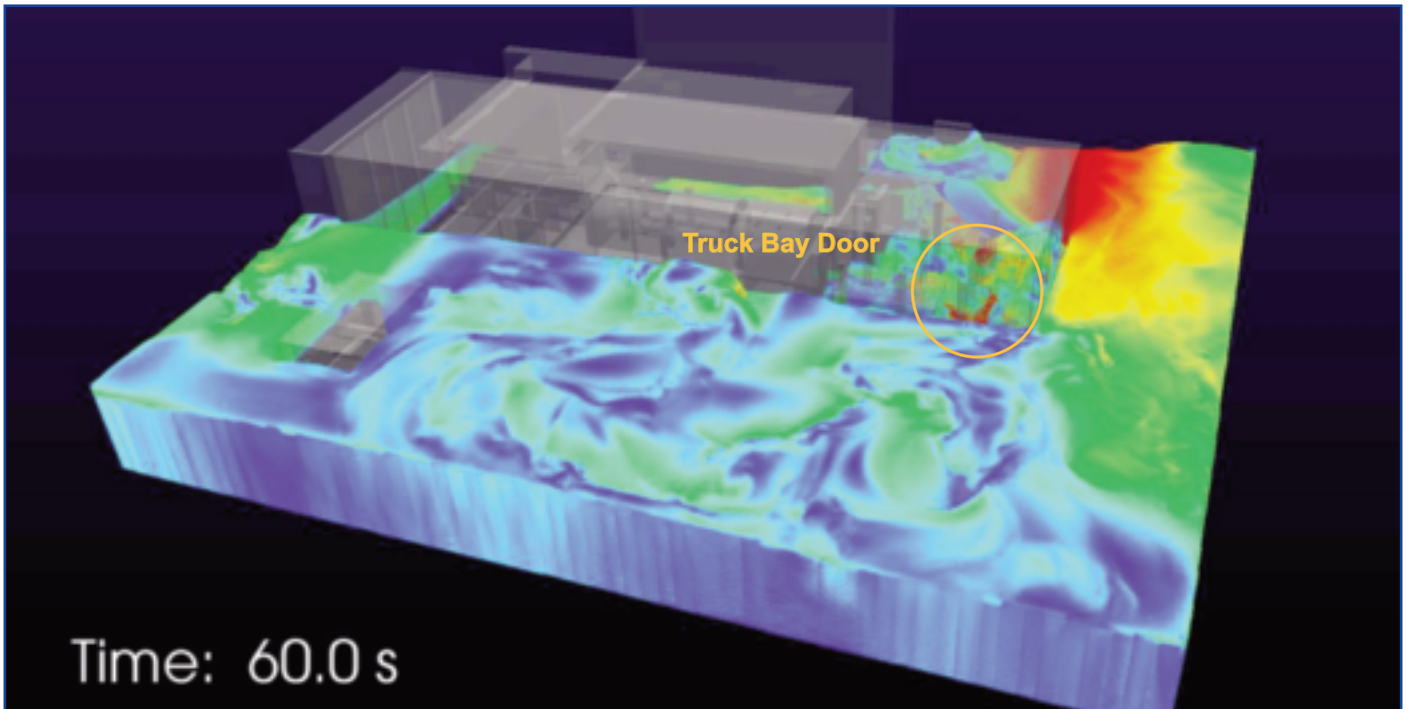
Deaeration from free surface in mixing tank with anchor blades



Next, flooding simulation in a turbine building of the plant was carried out. The boundary condition was made using the simulation result of the tsunami run-up simulation on the whole plant site. The track bay door was assumed to be broken at 40s due to a peak pressure. Seawater violently entered in the turbine building. Flooding was affected by the configuration of the rooms in the building. In this simulation, 130,000,000 particles were used with the size of 0.1m.

Figure 6:
Three-dimensional tsunami run-up simulation on Fukushima Dai-ichi Nuclear Power Plant by the Great East Japan Earthquake in 2011





Concluding Remarks

The MPS method is a powerful tool to analyze fluid flow with complex motion of free surfaces. It is now applied to some of the complex problems in industries, though further verifications and validations are required for more use.

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Figure 7:

Flooding analysis in the Turbine Building of Unit #1 of Fukushima Dai-ichi Nuclear Power Plant; the truck bay door is assumed to be broken at 40s

Computational Mechanics in South Africa (and Beyond)

by
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Most African countries have in place policies and action plans aimed at significant socioeconomic development in the next decade and beyond. Among key guiding documents is the Science, Technology and Innovation Strategy for Africa–2024, approved by African heads of state at an African Union Summit in 2014. African countries have recognized science and technology as the engine for development. So for example, a key target is that of achieving expenditure of 1% of GDP on research and development (GERD). By way of comparison, the 2013 average for the OECD countries is 2.4%.

commissioning of the Square Kilometre Array (SKA), which will be the world's largest and most sensitive radio telescope array.

This is a joint project between South Africa and Australia, with eight other African countries* as partners. The SKA project demands a dramatic increase in computational skills and resources, for modelling purposes as well as to manage and analyze the unprecedented volumes of data that will be generated. Nevertheless, the level of research in computational sciences broadly in Africa is quite low. While South Africa does boast capabilities that are at the cutting edge of research and which have strong links to high-tech industry, there is a clear recognition of the strategic need to expand and strengthen the computational sciences.

Perhaps the most striking example of scientific and technological progress in Africa has been the

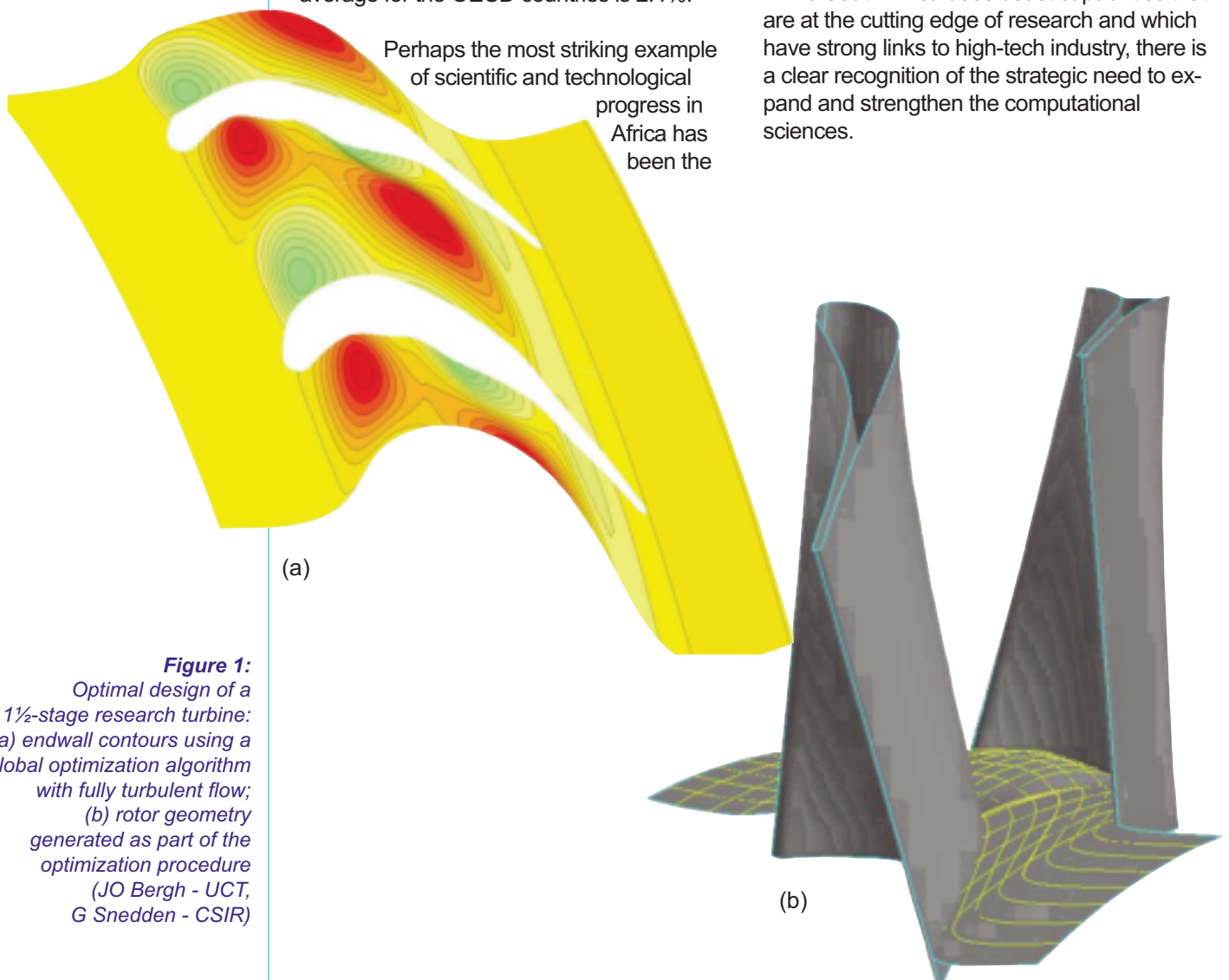


Figure 1:
Optimal design of a
1½-stage research turbine:
(a) endwall contours using a
global optimization algorithm
with fully turbulent flow;
(b) rotor geometry
generated as part of the
optimization procedure
(JO Bergh - UCT,
G Snedden - CSIR)

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CSIR

The Council for Scientific and Industrial Research (CSIR) of South Africa is a good example of an organization with a sustained R&D programme having significant components in computational mechanics, or multiphysics, and with strong links to national needs. Aeronautics at the CSIR has enjoyed the most intensive focus in this respect. Examples of research include the flow physics of accelerating and decelerating air vehicles, and integration and release studies for aircraft. Simulations of in-flight flutter excitation systems and flutter tests for clearance have supported light aircraft industries in South Africa, Europe and North America. A long-term research and development programme on the open source code OpenFOAM has proved its worth in the Aeronautic Systems Competency Area, and a significant outcome has been the development of a two-phase free-surface capturing scheme. This approach has been exceptionally successful in modelling violent liquid-gas sloshing validated with large-scale experiments. Other work has included the optimal design of turbine endwalls under turbulent flow conditions (Figure 1).

South Africa has some of the deepest mines in the world. There has been a long history of research in rock mechanics at the CSIR, with specific reference to problems in the mining industry. As an example of recent research, crack propagation models have allowed the simulation of dome cracks in the hanging walls of gold mines, some of which extend to just under 4km in depth. In recent years, the group has concentrated on acid mine drainage (AMD).

A biomechanical and blast wave modelling capability contributes to safety in sub-Saharan Africa, where the hazard of land-mines is still in existence. The Landwards group has used this capability in developing vehicles which survive land-mine blasts, and boots which provide protection to the legs and feet of soldiers.

The CSIR hosts the Centre for High Performance Computing (CHPC), which serves as a national facility. In addition to its national remit, the Centre is engaged in building high-performance computing capacity in a number of other African countries, in particular through their partnership in the Square Kilometre Array.

An equally important component is the availability of specialist computing expertise at the Centre. One of the major projects run at the CHPC concerns ocean-atmosphere

models of climate and climate change, from global Ocean General Circulation Models to regional scales of resolution.

The CHPC actively promotes high-performance computing among students, and has twice won the International Student Cluster Challenge hosted by the International Supercomputing Conference (ISC).

Computational Mechanics and The South African Research Chairs Initiative

The South African Research Chairs Initiative was established in 2006 as a strategic intervention of the South African government to increase research capacity and significantly expand the research base of South Africa in a way that supports international research and innovation competitiveness, while also responding to social and economic challenges of the country. Research Chairs may be established in any discipline: with just short of 200 currently in existence, around 10 have components in scientific computing and modelling, and two of these have a specific focus in computational mechanics: one in Industrial Computational Fluid Dynamics, and another in Computational Mechanics, both at the University of Cape Town (UCT).

The South African Research Chair in Computational Mechanics was awarded to the author in 2007. It is located at Cerecam (www.cerecam.uct.ac.za), a research centre which provides a coherent focus and point of interaction for research and applications in the general area of nonlinear multiphysics by promoting and supporting fundamental research, applied research, and industrial interaction. Its 14 members are permanent faculty in various branches of engineering, mathematics, physics, and biomedical engineering. The Chair has been instrumental in strengthening the activities in Cerecam, which is the only research centre in the country, and probably in sub-Saharan Africa, with a substantial international profile in computational mechanics. In addition to its research activities, Cerecam maintains a strong program in graduate studies, and has enduring links with a range of industries.

Activities in Cerecam span a broad range of topics. There has been a long-standing interest in problems of inelastic material behaviour, and this interest persists. In addition, there has been considerable growth in research activities relating to biomedical problems, the modelling of complex fluid behaviour, and the development and analysis of new finite element methods and algorithms.

“A major objective ... is ... promoting and developing computational mechanics on a continent in which the discipline is by and large significantly underdeveloped.”

Figure 2:
 A patient-specific FSI model for vascular access in haemodialysis:
 (a) arterio-venous shunt;
 (b) 4D MRI patient data;
 (c) simulation of the fistula
 (A de Villiers, AT McBride,
 BD Reddy (all UCT),
 B Spottiswoode
 (Siemens Medical Solutions USA))

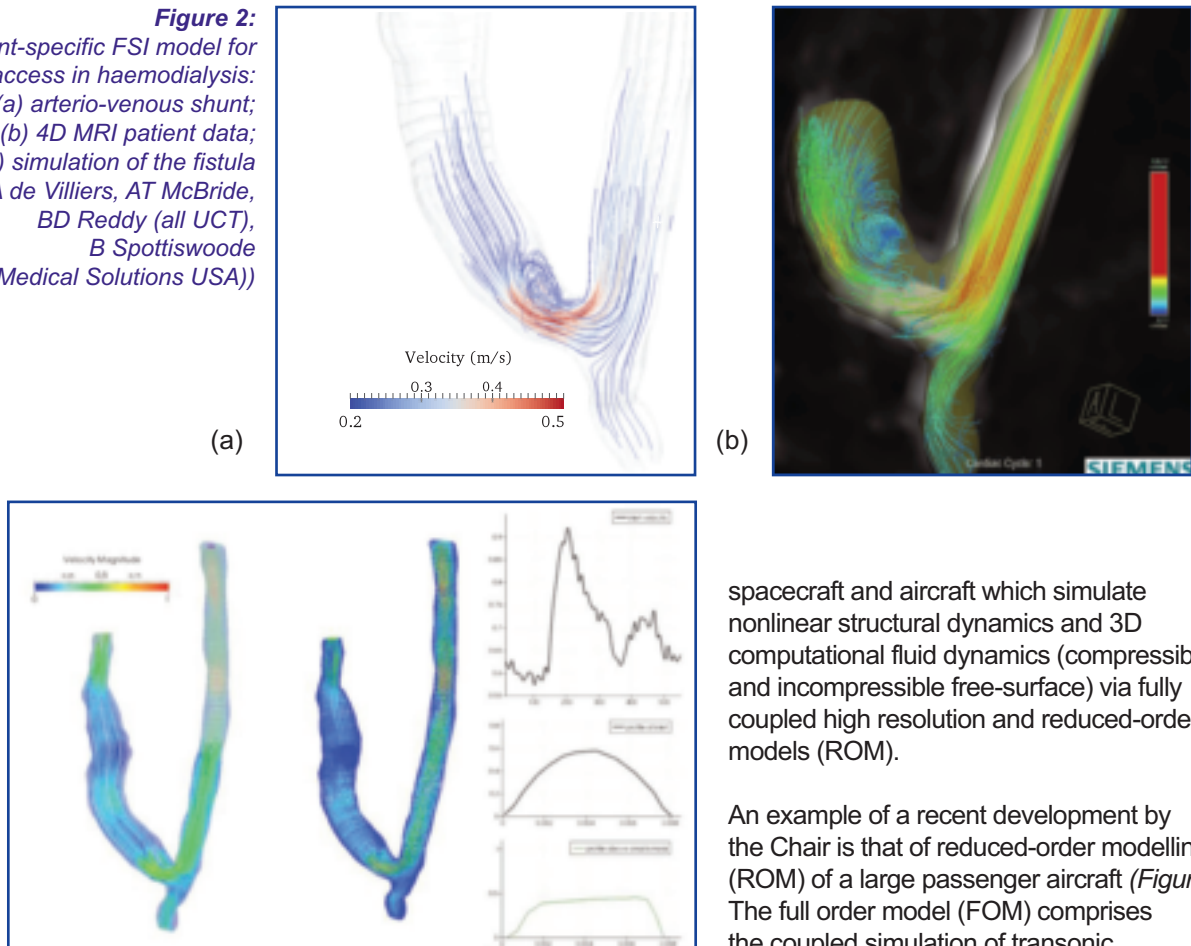


Figure 2 gives one example of current work, conducted in collaboration with colleagues at the University of Cape Town Medical School, on a patient-specific model for vascular access in haemodialysis.

The South African Research Chair in Industrial CFD, currently held by Prof. Arnaud Malan, was established with the aim of developing novel CFD modelling technology and expertise for the express support of industrially driven innovation. Partnerships with premier industries include Airbus (UK) and Airbus Defence & Space (Germany).

Activities in the Chair are focused on developing in-house algorithms and software that include comprehensive 3D models of

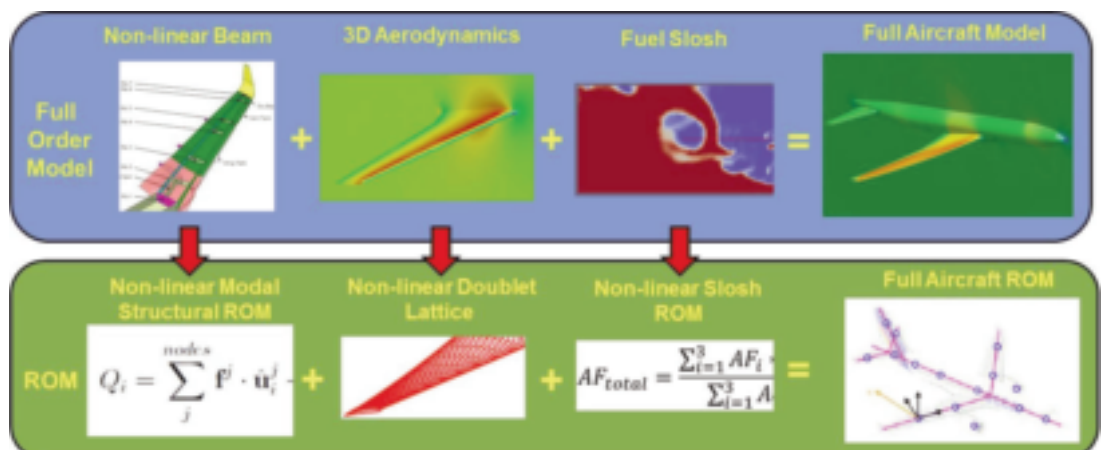
spacecraft and aircraft which simulate nonlinear structural dynamics and 3D computational fluid dynamics (compressible and incompressible free-surface) via fully coupled high resolution and reduced-order-models (ROM).

An example of a recent development by the Chair is that of reduced-order modelling (ROM) of a large passenger aircraft (Figure 3). The full order model (FOM) comprises the coupled simulation of transonic aerodynamics; wing and fuselage deflections via geometrically non-linear higher order finite element models; and violent fuel slosh with volume-of-fluid methods. The ROM is derived via processes that include proper orthogonal decomposition. This modelling technology has found applications in other areas such as water rocketry, where the CFD Chair led a project culminating in the setting of a new world record for a Class A Water Rocket.

National organizations and conferences

Before 1994, the Finite Elements and Computational Fluid Dynamics communities in South Africa held independent meetings, but in 1994 they joined forces to form the

Figure 3:
 Reduced-order modelling
 of aircraft dynamics
 (A Malan - UCT)



South African Association for Theoretical and Applied Mechanics SAAM (the word “saam” meaning “together”, in the Afrikaans language). SAAM represents the community at IACM and is also the national body that adheres to IUTAM, the International Union for Theoretical and Applied Mechanics.

SAAM has responsibility for organising the annual South African Conferences on Applied Mechanics (SACAM). These meetings bring together international speakers and southern African researchers from industry, the universities, and research organizations.

Computational Mechanics on the African continent

There has been a progress in establishing a series of African conferences along similar lines to existing regional meetings such as APCOM (the Asia-Pacific Conferences on Computational Mechanics), ECCOMAS, and the recently inaugurated PANACM (Pan-American Congress in Computational Mechanics). In 2009 the first African Conference on Computational Mechanics (Africomp) was hosted in Sun City, South Africa. The second meeting was held again in South Africa, this time in Cape Town in 2011. A concerted attempt has been made to ensure that the host centres rotate through the continent, and so it was pleasing that the third Africomp meeting took place 2013 in Livingstone, Zambia, which is located at Victoria Falls (Figure 4). This was followed by the 4th meeting, in 2015, which was held in Marrakech, Morocco.

The attendances at Africomp meetings have been small by the standards of the established regional meetings, but the quality of the scientific committees, plenary speakers, minisymposia, and contributed talks has been uniformly high. For example, at the Cape Town meeting there were 3 plenary and 12 keynote talks, and almost a hundred contributed papers by speakers from 22 countries in Africa, Asia, the Americas, and Europe. There has been a similar pattern at other Africomp meetings.

A major objective of Africom meetings is that of promoting and developing computational mechanics on a continent in which the discipline is by and large significantly underdeveloped. So for example, at the Livingstone meeting, faculty and students at three Zambian universities gained invaluable exposure to the world of computational mechanics by being involved in the local organization, and in addition by making it

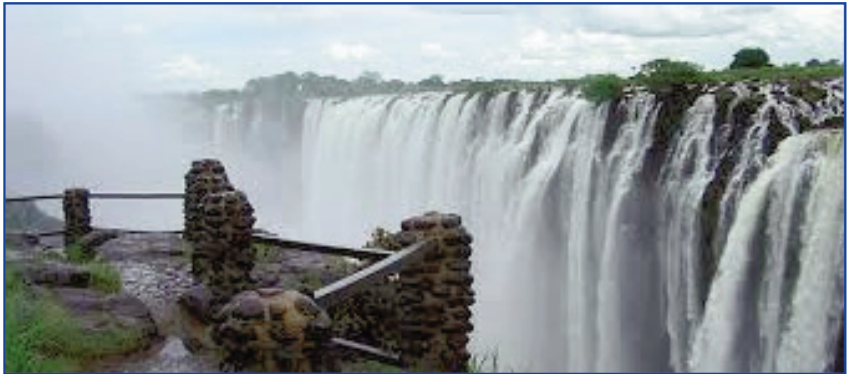


Figure 4:
(top) Some of the delegates at the 3rd Africomp meeting, Livingstone, Zambia;
(bottom) the nearby Victoria Falls

possible for graduate students and younger faculty from those universities to attend the conference, at no cost.

A further feature of the Africomp meetings has been the Zienkiewicz lecture, a plenary lecture delivered at the opening of the conference, and intended to honour the memory of OC Zienkiewicz, who passed away in January 2009, just days before the first Africomp Zienkiewicz lecture. This was delivered by Professor Tom Hughes, who also paid a warm and moving tribute to the memory of Olek Zienkiewicz, a pioneer and giant in the development of finite elements.

The Africomp meetings will continue, as a series endorsed by IACM. It is intended to strengthen future meetings by including as partners one or more computational mechanics organizations from outside the African continent. It is hoped that such partnerships will also promote the greater participation in Africomp by researchers from outside Africa.

Acknowledgement

The author is grateful to Arnaud Malan, Igle Gledhill, Glen Snedden, Jat du Toit, Jonathan Bergh, and Schalk Kok for contributions that were useful in writing this article. ●

Data-Driven Computing

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Computational mechanics has experienced tremendous growth over the past 50 years. Whereas the essential framework was established early on, several stubborn challenges have remained foci of extensive research to this day. One of those challenges is *material modeling*. Indeed, from the early days discerning computational mechanics understood that the fidelity of our material models is one of the main bottlenecks that limit the predictiveness of our codes. Indeed, the results of our simulations are only as good as the material models we employ, never better.

The search for better material theories and models for use in computation has been a truly intellectual endeavor that would not yield to brute force approaches. It naturally led to the consideration of the physics underlying material behaviour at increasingly smaller length and time scales. This is what we now call *multiscale analysis*, the material modeling paradigm of choice at present.

Simultaneously, the advances in *experimental science* over the past few decades have been equally phenomenal, including digital imaging, microscopy, diffraction methods, sensing and others. These advances have paved the way and provided impetus for the development of new theories of material behaviour and new computational paradigms, including multiscale modeling and simulation. They also have changed radically the nature of computational mechanics from a data-starved field to an increasingly data-rich field, which opens the way for the application of the emerging paradigm of *Data Science*.

Data Science is the extraction of 'knowledge' from large volumes of un-structured data^{1,2}. Data science often requires sorting through big-data sets and extracting 'insights' from those data. Data science uses analytics, data management, statistics and machine learning to derive mathematical models for subsequent use in decision making. Data Science currently influences primarily non-STEM fields such as marketing, advertising, finance, social sciences, security, policy, and medical informatics, among others. By contrast, the full potential of Data Science as it relates to scientific computing in general, and computational mechanics in particular, has yet to be realized.

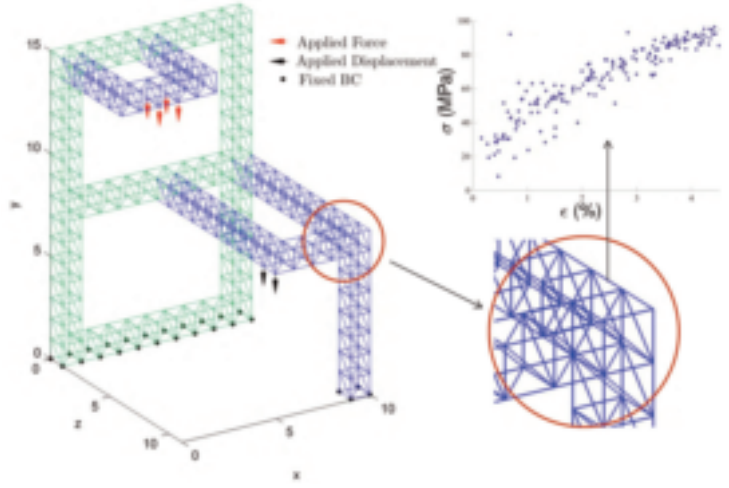
Boundary and initial-value problems in the physical sciences and engineering are different from those in the social sciences in that they have a great deal of mathematical structure. Thus, boundary and initial-value problems in science and engineering typically combine three types of equations:

i) *Conservation laws*, which derive from universal principles such as conservation of momentum or energy and are, therefore, uncertainty-free; ii) *Kinematics*, compatibility and essential constraints that relate local state variables, such as strains, to derivatives of field variables, such as displacements; and iii) *Material laws*, formulated through physical modeling based on experimental observation, that are, therefore, empirical and uncertain. The prevailing classical computational paradigm has been to calibrate empirical material models using observational data and then use the calibrated material model in calculations. This process of modeling a *fortiori* adds error and uncertainty to the solutions, especially in systems with high-dimensional phase spaces and complex behaviour. This modeling error and uncertainty arise from imperfect knowledge of the functional form of the material laws, the phase space in which they are defined, and from scatter and noise in the experimental data. Furthermore, often the models used to fit the data are *ad hoc*, without a clear basis in physics or a mathematical criterion for their selection, and thus the process of modeling is mired in empiricism and arbitrariness. Indeed, the entire process of empirical material modeling—and model validation thereof—is open-ended and no rigorous mathematical theory exists to date that makes it precise and quantitative.

The emergence of Data Science suggests a radically different scientific computing paradigm: Data-Driven Computing³, consisting of formulating calculations *directly* from material data, thus bypassing the empirical material modeling step of conventional computing altogether. In this new computing paradigm, essential constraints and conservation laws such as compatibility and equilibrium remain unchanged, as do all the numerical schemes used in their discretization, such as finite elements, time-integrators, *etc.* Such conservation laws confer mathematical structure to the calculations, and this mathematical structure carries over to the Data-Driven Computing

“With Data-Driven Computing, data sets can be used directly to provide predictive analysis capability for unmodeled materials.”

Figure 1: Three-dimensional truss structure containing 1,048 degrees of freedom. The detail shows a particular subset of bars in the structure and the inlay shows a typical data set describing the material behavior of each one of the bars



paradigm unchanged. However, in sharp contrast to conventional computing, in Data-Driven Computing the experimental material-data points are used directly in calculations *in lieu* of empirical material models. In this manner, material modeling empiricism, error and uncertainty are eliminated entirely and no loss of experimental information is incurred.

Specifically, Data-Driven Computing solvers seek to assign to each material point the state from a prespecified data set that is closest to satisfying the conservation laws and essential constraints. Equivalently, Data-Driven Computing solvers aim to find the state satisfying the conservation laws and essential constraints that is closest to the data set. The resulting Data-Driven Computing problem thus consists of the minimization of a distance function to the data set in phase space subject to the satisfaction of essential constraints and conservation laws.

We³ have investigated the performance of Data-Driven solvers in particular examples of application. *Figure 1* shows a test case consisting of a truss structure containing 1,048 degrees of freedom. The problem is to determine the equilibrium deformations of the truss under a combination of applied loads and boundary conditions. The truss undergoes small deformations and the material in all the bars is characterized solely by the data set shown in the figure.

The equilibrium constraints can be conveniently enforced by means of Lagrange multipliers. The corresponding stationarity equations correspond to the solution of two linear-static equilibrium problems for a comparison linear solid. A local data assignment iteration can then be performed by which each member of the truss is pegged to a particular point in the data set. The iteration terminates when the local state of every member of the truss is in the Voronoi cell of its assigned data point in phase space. The resulting Data-Driven solver possesses excellent convergence properties both with

respect to the number of data points and with regards to the local data assignment iteration. Our experience is that Data-Driven solvers are robust, reliable and provide a competitive alternative to the conventional model-driven computing paradigm.

The variational structure of Data-Driven problems confers additional robustness to the solvers and renders them amenable to analysis. By exploiting this connection, it can be shown³ that data-driven solutions converge to classical solutions when the data set approximates a limiting constitutive law with increasing fidelity. By virtue of this property, we may regard Data-Driven problems as a generalization of classical problems in which the material behaviour is defined by means of an arbitrary data set in phase space, not necessarily a graph. In particular, classical solutions are recovered precisely when the data set coincides with the graph of a material law.

The traditional computing paradigm has insulated problems from the data on which their solution is based. Removing this barrier creates a powerful new tool in the arsenal of scientific computing. With Data-Driven Computing, data sets can be used directly to provide predictive analysis capability for unmodeled materials. Traceability and inherent measures of data fidelity enable both deeper investigations into data-solution relationships and natural alerts for appropriate model use. Possessing the ability to tie solution results back to specific data points within a set establishes a new kind of data-causality in scientific computing. The Data-Driven Computing paradigm can also aid in the collection of representative data sets for prospective uses. Distance measures highlight data regions that require additional resolution, as well as point the analyst toward sensitivities within the solution-source relations. Tying the solution back to the data set also establishes an elegant way of limiting model accuracy to the resolution of the source data. Additionally, it bears emphasis that material models typically have specific regimes over which they are developed. However, the models themselves are easily used outside their intended range. Especially with regards to empirical *ad-hoc* curve fits, such overreach can neither be justified nor easily prevented. By directly using a data set in calculations, attempts to simulate beyond the data regime are met and penalized by large calculated distance metrics, regardless of how the user receives the data set. These tangible and intangible benefits add considerable appeal to Data-Driven Computing and flag it as an exciting emerging field worthy of further investigation. ●

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Advanced Computational Methods to Understand & Mitigate Extreme Events

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Extreme events are situations where the loading and/or response of a material, structure, or system exceeds that of normal conditions. They can be naturally occurring or man-made, and they cross essentially all disciplines of science and engineering. These problems often define the research boundaries for science and technology in the sense of our ability to predict, analyze, and mitigate their effects. Examples include earthquakes, landslides, explosions (Figure 1), projectile penetration, and hypervelocity space impact, to name a few.



Figure 1:
 Large-scale explosion, an example of an extreme event (courtesy of U.S. Army ERDC)

In the field of extreme events research, physical experimentation is often limited according to the high rates, short time scales, large deformation response and/or physical size that are inherently present in these problems. Computation extends our capabilities beyond these experimental limitations, however methods suitable for modeling these events must be versatile and stable when dealing with:

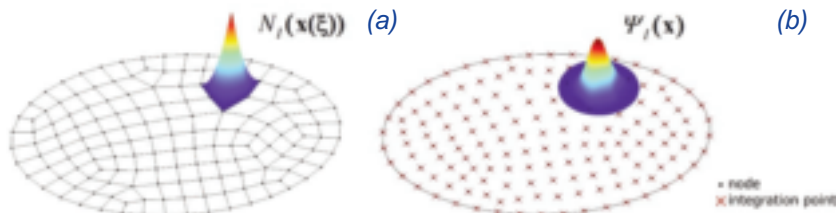
- rough solutions in the form of transient strong discontinuities (fractures) and weak discontinuities (localization)
- severe material deformation and material instability
- multi-body contact without a priori knowledge of potential contacting bodies and contact surfaces
- multiple, evolving, and mixed length scales
- multiple and coupled physics

Meshfree methods such as the reproducing kernel particle method (RKPM) [1,2] offer unique features that are particularly attractive for modeling extreme events. By employing these methods, the domain can be

discretized by a set of scattered nodes, and the approximation is constructed directly in the Cartesian coordinates with only nodal information. As seen in Figure 2, rather than a structured mesh defining connectivity as in the conventional finite element method, the interaction between points is achieved through the nodes' kernel coverage of any point in the domain. Consequently, issues related to mesh distortion, entanglement, alignment, and so on, are greatly relieved or completely circumvented. Adaptive refinement is also made easier as the conforming condition is relaxed to the partition of unity subordinate to open covering of the domain. The continuity of the approximation is entirely independent of the order of basis functions, allowing arbitrary smoothness (and roughness) in the approximation to be varied in space and time according to the physics of the problem at hand. Essential features such as crack-tip singularities and strong discontinuities can also be embedded in the approximation through intrinsic enrichment. The resulting purely node-based discretization is suitable for problems with damage, material flow, complex evolving multi-body contact, and fragmentation [3].

Figure 2:

- (a) Construction of finite element shape functions by patching local element domains;
 (b) Reproducing kernel shape functions constructed directly in the Cartesian coordinates with direct nodal integration scheme



Weak-form based meshfree methods necessitate numerical quadrature. Nodal integration, as shown in Figure 2(b), is a natural choice for this class of problems, as it is particularly advantageous for modeling material failure, fracture and separation that typifies extreme events. However, nodal integration constitutes low order quadrature and can yield poor accuracy. As seen in Figure 3(a), the solution to PDEs by direct nodal integration (DNI) does not

converge with refinement of non-uniform discretizations. Based on the framework of variational consistency [4], the variationally consistent integration (VCI) method has been introduced as a correction of any given quadrature to restore accuracy and optimal convergence. The method can be used to correct nodal integration methods such as DNI, stabilized non-conforming nodal integration (SNNI) [3] (the non-conforming version of stabilized conforming nodal integration [5]), and 2nd order Gauss quadrature (GI-2) to yield convergent solutions, as seen in Figure 3(a).

While most natural for modeling material damage under extreme conditions, nodal integration is also subject to instability due to the severe underestimation of the strain energy of short-wavelength modes. As shown in Figure 3(b), strains vanish at nodal locations for modes with a wavelength of two times the nodal spacing. As a consequence, they can grow virtually unbounded and destroy the numerical solution as seen in Figure 3(c) where Poisson’s equation is solved using DNI for illustration. Naturally stabilized nodal integration (NSNI) [6] has recently been introduced to circumvent this difficulty, and also address other shortcomings in nodal integration for modeling extreme events. The method yields stable solutions as shown in Figure 3(d), where Poisson’s equation is solved using NSNI. The method is based on the Taylor expansion-type stabilization that originated in finite elements [7], but employs implicit gradients [8] rather than direct derivatives in the expansion. NSNI can be employed in conjunction with VCI to yield a method that is stable, convergent, and efficient [6]. The method is free of conforming cells and background meshes, and is thus suitable for modeling extremely large deformations encountered in extreme events.

Many extreme events involve complex failure mechanisms across multiple length scales. A micro-crack informed damage model for describing the softening behavior of brittle solids has been proposed [9], in which the damage accumulation is treated as a consequence of micro-crack evolution.

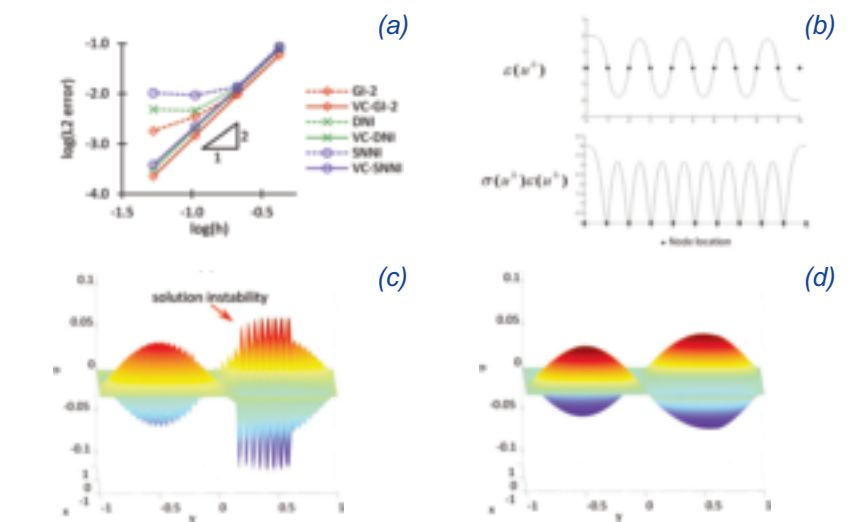
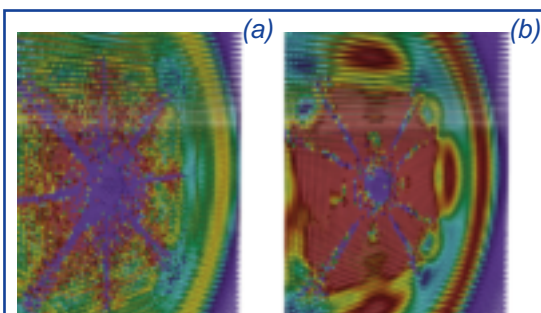
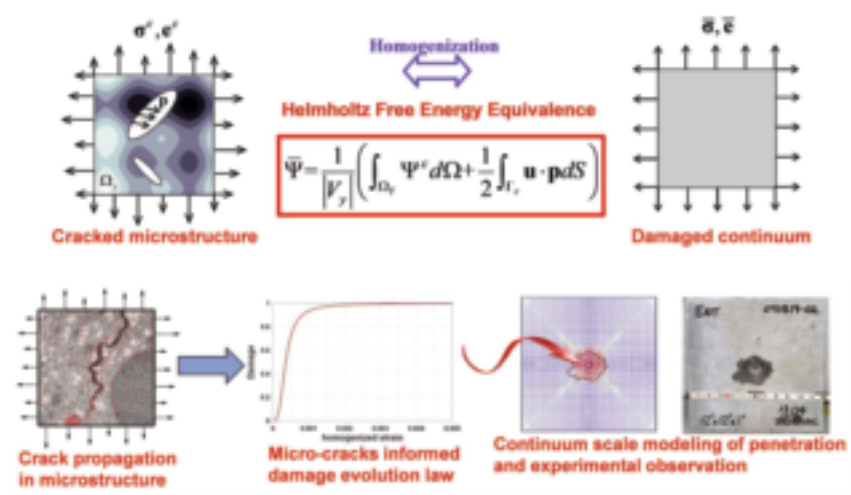


Figure 3: Convergence of several low order quadrature schemes in a non-uniform discretization of $\Delta u + \sin(\pi x) \sin(\pi y) = 0$ on Ω , $\Omega: (-1, 1) \times (-1, 1)$, $u = 0$ on $\partial\Omega$; “GI-2” 2x2 Gauss integration, “DNI” direct nodal integration, “SNNI” stabilized non-conforming nodal integration, prefix “VC-” variationally consistent; (b) Examination of strain energy associated with an oscillating displacement mode $u^h(x) = \sum_{L=1}^{NP} \Psi_L(x) u_L$, $u_L = (-1)^L$; Solution to $\Delta u + \sin(\pi x) \sin(\pi y) = 0$ on Ω , $\Omega: (-1, 1) \times (-1, 1)$, $u = 0$ on $\partial\Omega$: (c) Solution by direct nodal integration, and (d) Solution by NSNI

The Helmholtz free energy in the cracked microstructures is made equivalent to that of the damaged continuum as shown in Figure 4(a), such that the micro-scale fracture models and the continuum-scale damage models exhibit equivalent energy density dissipation. This approach has been applied to fragment-impact modeling of concrete structures [10], and is shown in Figure 4(b).

Figure 4. (a) Micro-crack informed damage model [9]; (b) multi-scale modeling of material damage [10]



To illustrate the effectiveness of these methods, a suite of penetration problems from the blind prediction study in [11] is examined with SNNI [3] (a nodal integration) and NSNI [6] (a stabilized nodal integration). The problems

Figure 5: Von Mises stress in concrete penetration: (a) SNNI and (b) NSNI.

Figure 6:
Cross-section of a penetration process using (a) SNNI, and (b) NSNI

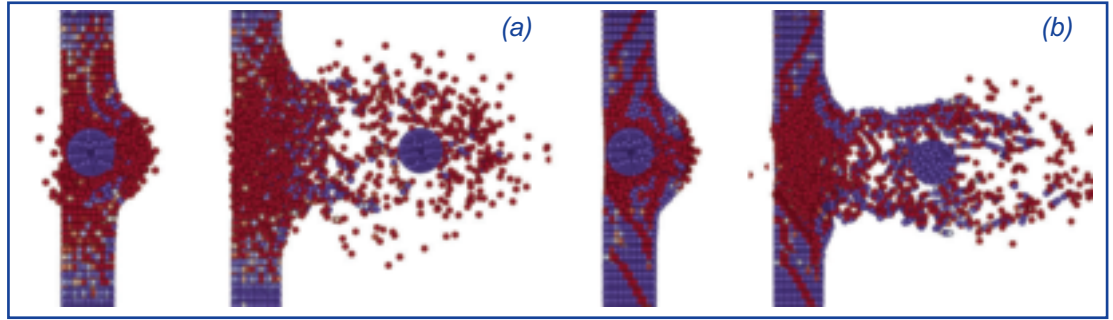


Figure 7:
Top to bottom: exit face damage, impact face damage. Left to right: experiment, SNNI, and NSNI

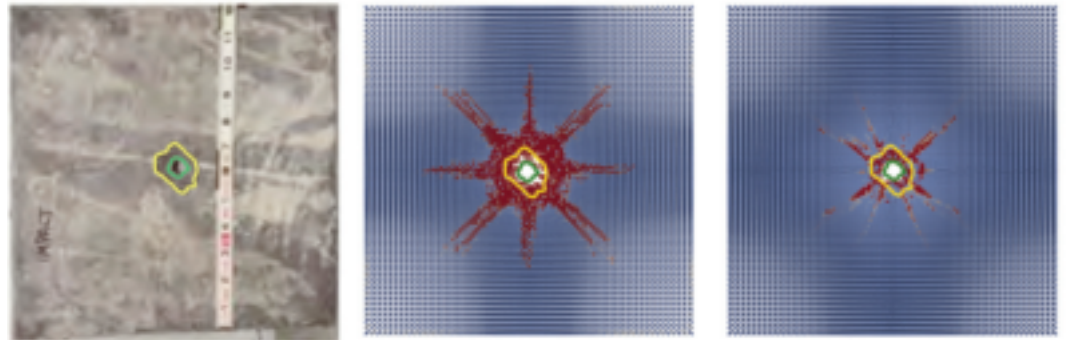
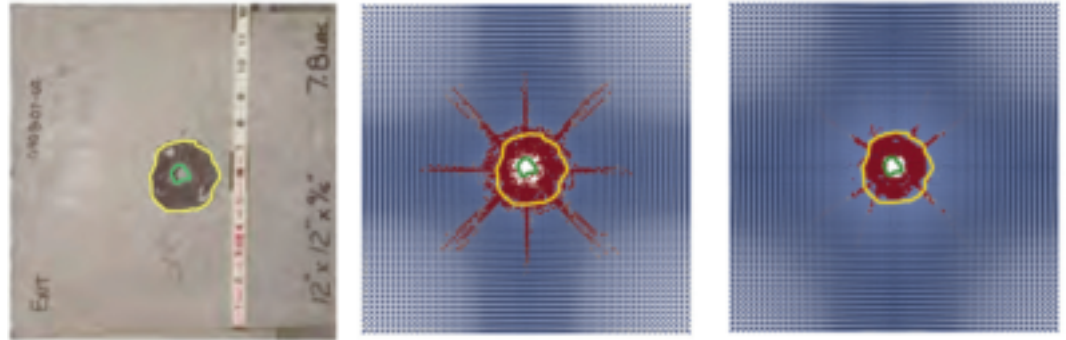


Figure 8:
(a) Numerical by NSNI and experimental [13] cracking patterns; Top: cross sections of the cracking pattern at the point of impact, Bottom: cross sections of the cracking pattern away from impact; (b) Top: lateral cracking in numerical simulations, Bottom: lateral cracking in a brittle impact experiment [14].

in this study are representative of one of the many difficult classes of problems in the field of extreme events. Penetration of CorTuf concrete [12] panels with varying thicknesses and impact velocities is simulated. Figure 5(a) shows the von Mises stress from an SNNI simulation of

the penetration process; checker-boarding, a multi-dimensional version of one-dimensional oscillating modes, is clearly observed in the stress field when pure nodal integration is employed. This results in unreasonable debris cloud shapes, and excessive, diffuse damage, as seen in

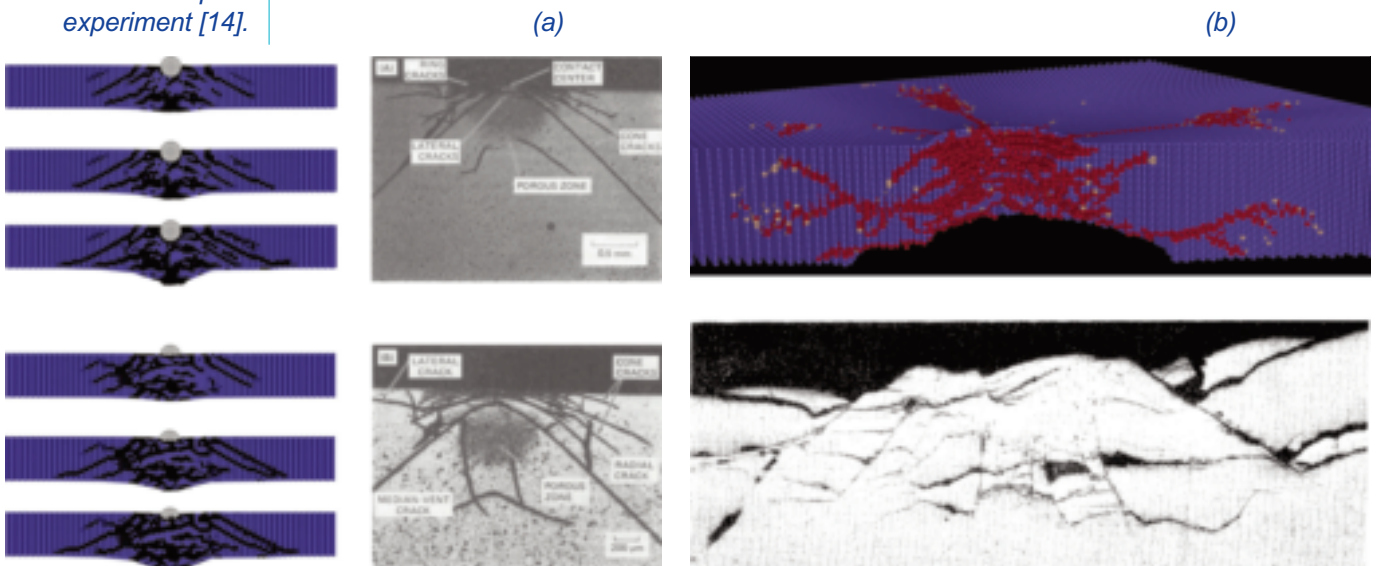


Figure 9:
Fragmentation of concrete target in a perforation event with large velocity reduction of the penetrator

Figure 6(a).

As a consequence, the expected shear-cone formation is almost completely absent for the SNNI solution, and the predicted crater and hole sizes are considerably larger than the experimental results (Figure 7). In Figure 5(b) it is seen that the stability of NSNI avoids spurious checker-boarding, and captures clear radial cracking. Subsequently, shear-cone formation is captured when NSNI is employed as shown in Figure 6(b). The NSNI results also show much better agreement with the experimental failure patterns in Figure 7.

The radial and lateral cracking patterns obtained by NSNI are in agreement to those experimentally observed in brittle material failure, as shown in Figure 8. The change in the dominant failure mode as a function of penetration conditions is observed in NSNI simulations as shown in Figure 9 and Figure 10. For the case in Figure 9 where there is a large velocity reduction of the penetrator i.e., the penetrator is nearly stopped by the target, and large pieces of intact debris are formed as the penetrator perforates the target, which is consistent with experimental observations. For cases where the penetrator overmatches the target and maintains significant exit velocity, the excessive kinematic energy is dissipated via high density material damage leading to debris cloud formation; qualitative agreement between experimental results and NSNI simulations is shown in Figure 10.

This computational framework can also be used to model impact and blast loads on ductile materials, where the ductile failure modes are properly captured. Figure 11 shows a steel plate subject to a blast load from the UC San Diego blast simulator [16]. It is seen that the formulation captures the large ductile deformation and tearing at the edge

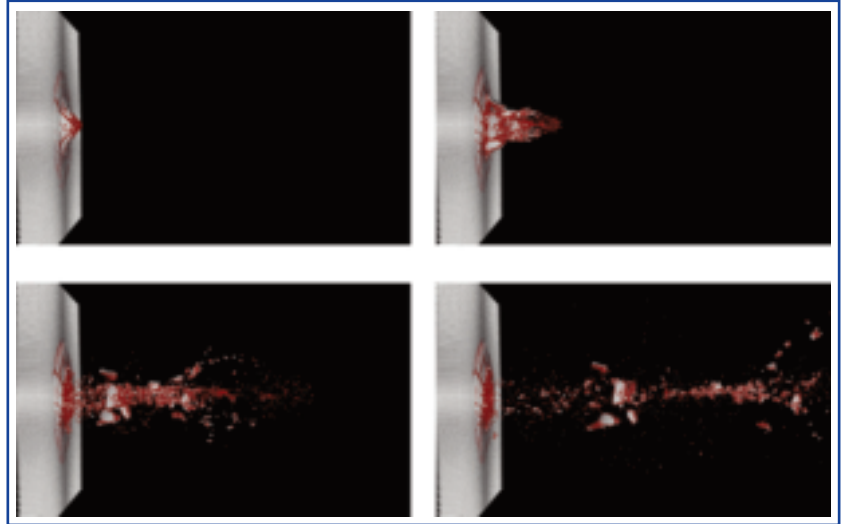


Figure 10:
Comparison of debris cloud in perforation of concrete target with moderate reduction in penetrator velocity:
(a) Numerical, (b) Experimental [15]

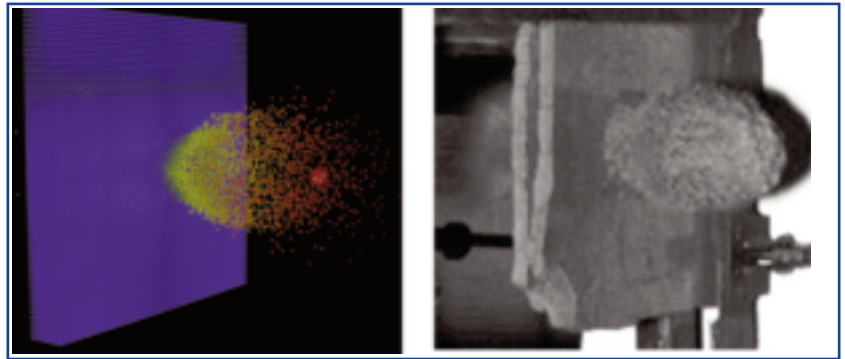


Figure 11:
Evolution of a steel plate subject to a load from the UC San Diego blast simulator [16]

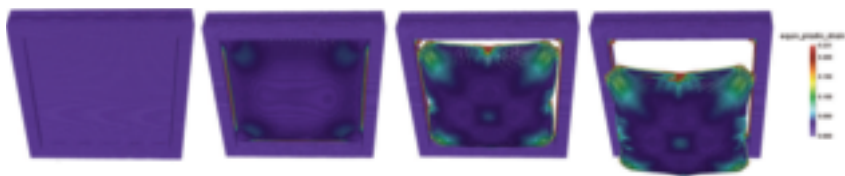
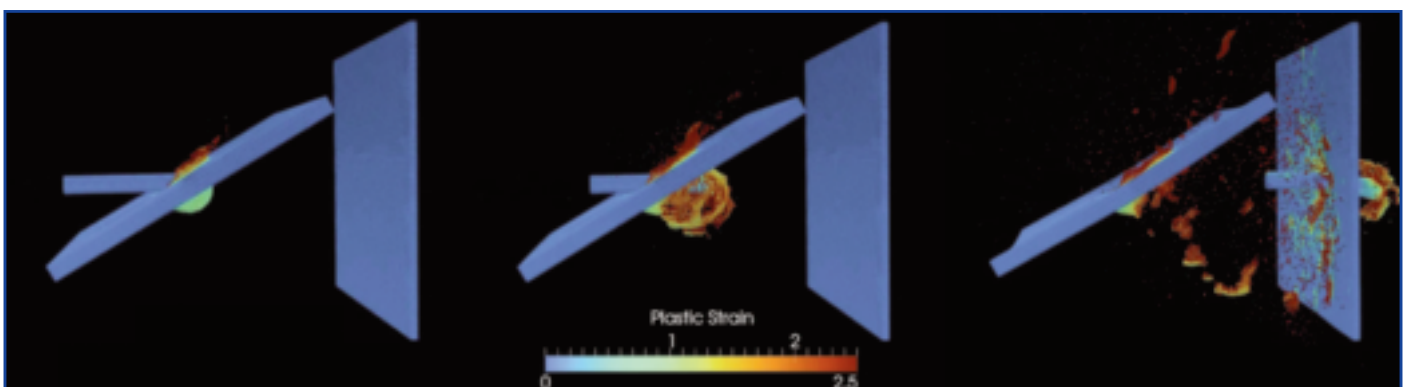


Figure 12:
Evolution of multi-layer impact problem with behind-armor debris field



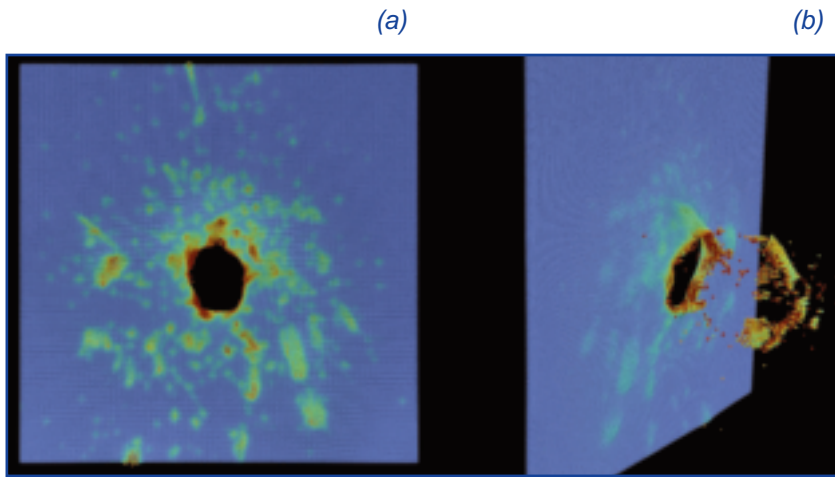


Figure 13:
Simulation of multi-layer impact with behind-armor debris field:
(a) front of witness plate: debris impact damage on second plate;
(b) back of witness plate: rod perforation of second plate and additional debris field.

of the reaction support frame. *Figure 12* and *Figure 13* show the simulation of a tungsten rod penetrating an oblique steel impact plate backed by a thin aluminum witness panel. A variety of penetration mechanisms and damage modes associated with ductile material failure are seen, where large plastic deformation, tearing, penetrator bending and debris field interaction are evident. In this class of problems, finite element techniques for penetration such as erosion would be ineffective at capturing the behind-armor debris; evaluating the safety of humans inhabiting a protective structure would not be possible. *Figure 14* shows the evolution of a landslide simulation with clear capturing of shear band formation, material flow, and shearing failure modes. ●

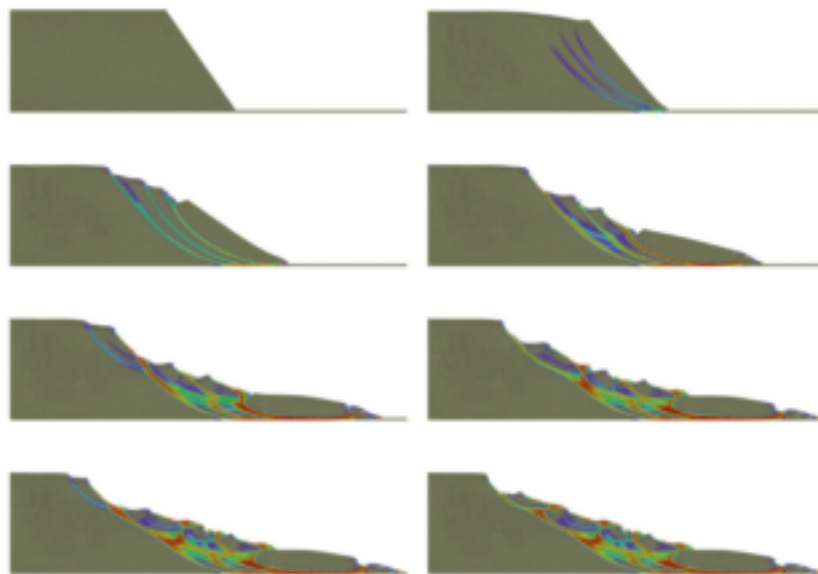
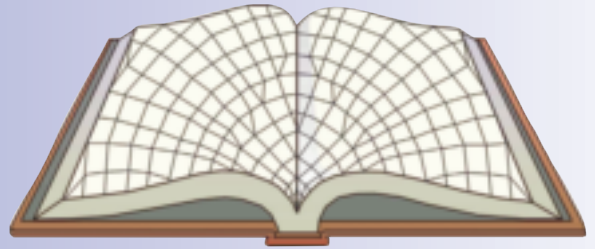


Figure 14:
Top left to bottom right:
evolution of a landslide simulation using NSNI-RKPM.

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A FINITE ELEMENT PRIMER FOR BEGINNERS: THE BASICS



Tarek I. Zohdi

Springer, London, UK, 2015

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Contents: Preface; 1: Weighted Residuals and Galerkin's Method for a Generic 1-D Problem; 2: A Model Problem: 1-D Elastostatics; 3: A Finite Element Implementation in One Dimension; 4: Accuracy of the Finite Element Method; 5: Element-by-Element Iterative Solution Schemes; 6: Weak Formulations in Three Dimensions; 7: A Finite Element Implementation in Three Dimensions; 8: Accuracy of the Finite Element Method; 9: Time-Dependent Problems; 10: Summary and Advanced Topics; Appendix A: Elementary Mathematical Concepts; Appendix B: Basic Continuum Mechanics; Appendix C: Convergence of Recursive Iterative Schemes.

As the title implies (in three different ways!), this nice little book is an elementary introduction to the Finite Element Method (FEM). I like short books like this, which introduce the essence of a topic to the reader in a hundred or so pages. Another such book which I read many years ago is "A Multigrid Tutorial" by W.L. Briggs, from 1987, which contains 90 pages, and is a delightful introduction to the Multigrid method. Then in 2000, a second edition of that book was published, with two additional authors, and with about twice as many pages. The whole charm of the original book was gone! The original simple and concise exposition has drowned in a sea of details. I am not even sure if I would have bothered with it back then, had the second edition fallen into my hands first. Of course, now the original version is out of print...

The book by Zohdi, which has a printed version and an electronic version, discusses the FEM for 1D and 3D problems in linear elasticity. Everything is written concisely, and many details are omitted, but this fits well the lean format of the Springer Briefs series to which this book belongs. The book looks attractive and is easy to read.

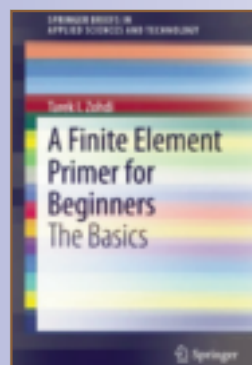
Chapter 1 introduces the ideas behind Weighted Residual methods and the Galerkin method. The motivation given here to Galerkin's method, which I have not seen in other books, is particularly nice. First, we approximate the exact solution by a series of the form

$$u^N = \sum_{i=1}^N a_i \phi_i(x), \quad (1)$$

where the functions ϕ_i are the chosen basis functions which span the approximation space. Now, we wish the approximate solution u^N to be the projection of the exact solution on the approximation space, since in this way we will get the minimal error. See Figure 1.



Tarek Zohdi



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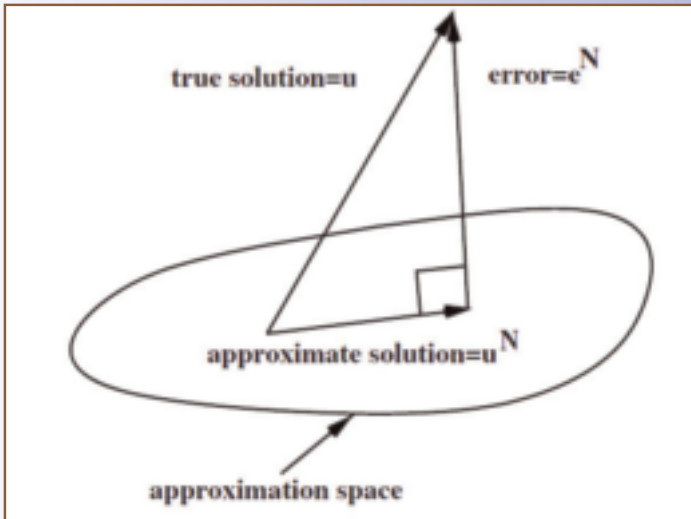


Figure 1:
Orthogonality of the approximation error.
 This is Fig. 1.1 from the book.

Therefore, we want the error to be orthogonal to the approximation space, i.e.,

$$\int_{\Omega} e(x) \phi_i(x) dx = 0, \quad (2)$$

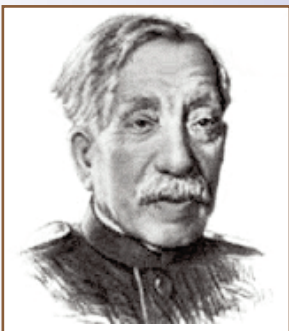
where Ω is the computational domain, and e is the error. Unfortunately, eq. (2) is useless as a practical requirement, since we do not know the error e ! So instead of the error, we will take the next best thing to the error, namely the *residual*, which is a quantity we can actually compute. Thus, we replace (2) with the requirement

$$\int_{\Omega} r(x) \phi_i(x) dx = 0, \quad (3)$$

where $r(x)$ is the residual of the differential equation. Substituting the expression for the residual $r(x)$ and using (1) give us (after some additional manipulations) the Galerkin method.

Of course, in the Galerkin method the error *is* orthogonal to the approximation space after all, although not in the L_2 inner-product as implied by (2), but in the energy inner-product. This is not pointed out in *Chapter 1*, and wisely so, since the reader is not yet ready to digest all this. The orthogonality in the energy norm is proved later, in *Chapter 4*.

The exposition described above is abstract, and therefore will be easily accessible to a reader who is mathematically oriented. A reader who is less so, or has never heard of basic functional analysis concepts, such as the projection of a function on a space of functions, would find the exposition a bit harder to absorb. It would have been a good idea to include such concepts in Appendix A. Of course, with an appropriate guidance in class, this should not pose any difficulty.



Boris Galerkin

Another nice discussion is included in *Chapter 2*, on the weak form of the 1D problem. The author explains the matter of smoothness, and the terms “strong” and “weak”. This explanation is missing from most books on FEM. The book from which I first studied FEM as a student proved that the strong and weak forms of the problem are equivalent, and I remember wondering in what way the strong form was “stronger” than the weak form if they were indeed equivalent.

Chapter 2 ends with some comments on material nonlinearity. This provides a glimpse into nonlinear FE formulations, while the book generally covers only the linear case. *Chapter 3* discusses the FE implementation in 1D. Simple examples which can be solved “manually” are given in order to demonstrate the techniques. Section 3.9.4 briefly talks about the saving in storage as the advantage in the sparse structure of the global stiffness matrix. The saving in computing time, which is generally regarded as more critical, is not mentioned here, but is mentioned in *Chapter 7*, in the context of the FE implementation in 3D.

Chapter 4, which discusses the accuracy of FEM, includes a proof of the principle of minimum potential energy, as the infrastructure used for the Rayleigh-Ritz method. More precisely, the discussion connects between this principle and the weak form of the problem. This is done here in two ways: by an elementary calculation, and by the calculus of variation. The double derivation is nice, as in most books only one of them is provided, if at all.

Chapter 4 also explains, in a simple and clear way, how one can estimate the error constant C and find the mesh parameter h which would provide a desired level of accuracy. In addition it gives a nice mathematical basis to the use of the residual as an indicator in local adaptive refinement schemes.

Chapter 5 discusses iterative schemes for the solution of the linear system of algebraic equations, namely steepest descent (SD), conjugate gradients (CG), an pre-conditioned CG. The SD and CG methods are first derived and then written as formal algorithms, ready for implementation.

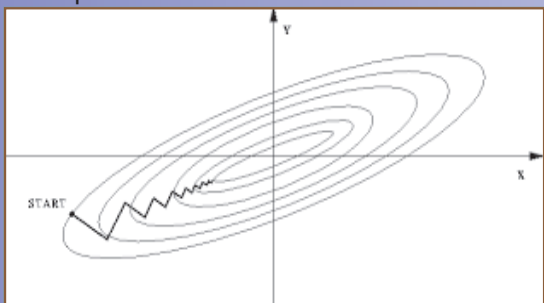
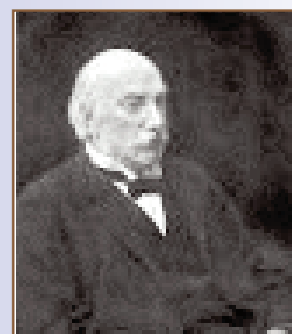


Figure 2:
 Typical progress of the minimization in the SD method.
 Taken from the thesis of T. Hjorteland, University of Oslo, 1999.



The Lord Rayleigh

Chapters 6-8 are the 3D analogs of chapters 2-4. Special topics which appear here for the first time include the principle of complementary energy (Chapter 6), where the discussion is limited to the continuous level, and a *posteriori* recovery methods (Chapter 8), briefly presenting the basic idea.

Chapter 9 deals with time-dependent problems in linear elasticity. The discretization process is presented in a non-standard way: first the PDE is discretized in time, and only then the resulting semi-discrete equations are discretized in space by FEs. Of course, the final result is the same as in the standard approach. The time-stepping method presented is the Generalized Trapezoidal (GT) method for a first order system. To this end, the elastodynamics equations are cast in first order form, with the displacements and velocities as independent unknowns. This is equivalent to the standard way in which GT is applied to the first-order system



Walther Ritz

$$\begin{bmatrix} 0 & M \\ I & 0 \end{bmatrix} \begin{Bmatrix} \dot{d} \\ \dot{v} \end{Bmatrix} + \begin{bmatrix} K & 0 \\ 0 & -I \end{bmatrix} \begin{Bmatrix} d \\ v \end{Bmatrix} = \begin{Bmatrix} F \\ 0 \end{Bmatrix} \quad (4)$$

with obvious notation. Forward Euler (explicit) and Backward Euler are presented as special cases.

One may wonder whether it would not have been better to introduce the Newmark method, which is a more standard time-stepping method for problems in elastodynamics. I support the author's choice in this case. The advantage of GT is that it is very simple to present and understand, while introducing the Newmark method would be much more involved. We have to remember the purpose of this book and its elementary style. The author does direct the reader to several other books for further reading.



Leonhard Euler's image on a Swiss Franc bill

Chapter 10 briefly discusses concepts related to domain decomposition and parallel computing. Three appendices follow, which cover concepts from mathematics, continuum mechanics and iterative schemes.

Unfortunately, the book contains many typographical errors, but the reader can avoid confusion by consulting the errata page posted on <http://cmrl.berkeley.edu/zohdipaper/ERRATA-FOR-ZOHDI-FEM-BOOK.pdf>. Hopefully a second and corrected edition will be published soon.

In summary, this is a nice little elementary book on FEM, which has an attractive and non-intimidating form for the student beginning her/his FEM studies, or for individuals whose area of interest is different but desire to get a taste of what FEM is all about. This book certainly provides this "taste", and does it effectively. ●



From ACME to UKACM: a new name for 2016

for all inclusions under
UKACM

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The Association of Computational Mechanics in Engineering in the United Kingdom (ACME-UK) was founded in March 1992 to promote research in Computational Mechanics in the UK and to establish formal links with similar organisations in Europe and the rest of the world. At the start of this year the association changed its name to the UK Association for Computational Mechanics (UKACM) to move in line with many other associations, and also to improve the all-important web presence (you can find the UKACM webpages at www.ukacm.org).

UKACM continues to be the single UK body affiliated to the European Community of Computational Methods in Applied Sciences (ECCOMAS) and the International Association for Computational Mechanics (IACM). Another major change from the start of 2016 was the Presidency passing from Prof. Carlo Sansour, of Nottingham University to Prof. Charles Augarde, of Durham University. UKACM is administered by an Executive Committee, with officers Prof. Omar Laghrouche (Treasurer), Prof. Akbar Javadi (Secretary) and Dr Rubén Sevilla (Web).

Report on the 24th ACME conference

by:
Prof. Tony Jefferson,
Dr Pierre Kerfriden,
Dr Iulia Mihai,
Dr Susanne Claus
ACME 2016
Organising Committee

The principal activity of UKACM is 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 aimed at PhD and Post-Doctoral researchers, who are encouraged to present their latest research in a friendly environment. For the last five years the conference has been preceded by a 'School' that aims to provide teaching to PhD students and Post-Doctoral researchers on a computational theme of interest.

This year the conference was hosted by Cardiff University and held in the University's main building on Park Place between 30th March and 1st April. This was the second time Cardiff had hosted the conference, with the previous occasion being in 2004. The conference was preceded on the afternoon of March 30th by the 5th ACME School, on the subject of 'Computational Modelling Through the Scales'. The 100 delegates who attended the School were informed and entertained by lectures from Pierre Kerfriden on multi-scale modelling and by Tony Jefferson on micro-mechanics and its use in developing constitutive models. The lecturers found the audience engaged, attentive and almost constantly awake, for which they were most grateful.

The main conference commenced with an opening ceremony on the morning of 31st March that included brief presentations from the conference chairs, Prof Sam Evans (the Director of Cardiff School of Engineering) and Prof Charles Augarde (UKACM President). During this ceremony, delegates were reminded, via a canine analogy, of the conference's ethos of being friendly, supportive, helpful and constructive. The organisers are pleased to report that the 131 delegates who attended the conference

Figure 1:
Conference delegates



maintained this ethos throughout. These delegates came mostly from UK universities, although a few had travelled from more distant climes.

The conference proceedings comprise 104 four-page extended abstracts on a variety of subjects, including geomechanics, coupled problems, failure & damage, fluid mechanics, electro-magnetics, material modelling, biomechanics, optimisation and solids & structures (see the UKACM website to download the proceedings). Presentations were distributed among five parallel sessions and the organisers were particularly impressed by the quality of the presentations and of the scientific work presented. The organisers would especially like to thank all of those who acted as session chairs and for keeping the sessions to schedule.

The conference included four excellent plenary lectures, which were given by Professor Antonio Huerta from UPC Barcelona, Prof. Anthony Gravouil from L'Université de Lyon, Prof. Bert Sluys from TU Delft and Dr Garth Wells from Cambridge University. All of the plenary lectures were very well received and the organisers are extremely grateful to the plenary speakers for their inspirational talks.

Cardiff's famous castle was the venue for the conference banquet. This event was notable for its conviviality, lack of speeches and for the magnitude of the wine bill. At the brief closing ceremony, many people were thanked for their hard work before and during the conference. Particular gratitude was expressed to Samantha Emmott, from Cardiff University's conference office, Cardiff PhD students, who helped with the Audio Visual equipment in the lecture rooms, all presenters and to the UKACM Exec. Committee for their help and support.

We, the main organising committee, comprised Dr Iulia Mihai (Lecturer at Cardiff), Dr Susanne Claus (Ser Cymru Research Fellow) and the conference chairs, Dr Pierre Kerfriden and Prof. Tony Jefferson. We enjoyed organising this conference together but equally feel a relief that it is now in the past. We bid farewell to this, the final ACME conference and eagerly await the first UKACM conference, to be hosted by Dr Asaad Faramarzi at Birmingham University, where we will enjoy being unstressed delegates. We wish Asaad well in his preparations for next year's event (see ukacm2017.ukacm.org/ for details of the 2017 conference).

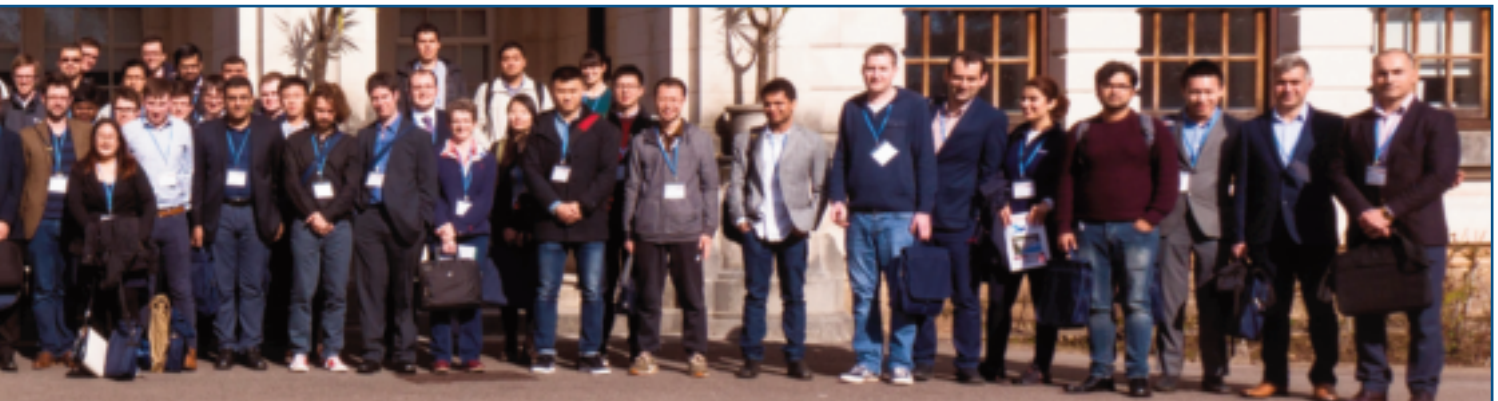
ACME Conferences over the years:

2016: Cardiff University	2008: University of Newcastle	1999: Durham University
2015: Swansea University	2007: University of Glasgow	1998: Exeter University
2014: University of Exeter	2006: Queen's University Belfast	1997: Imperial College, University of London
2013: Durham University	2005: Sheffield University	1996: Glasgow University
2012: University of Manchester	2004: University of Wales, Cardiff	1995: Oxford University
2011: Heriot-Watt	2003: University of Strathclyde	1994: Manchester University
2010: University of Southampton	2002: University of Wales, Swansea	1993: University College of Swansea, Wales
2009: University of Nottingham	2001: Birmingham University	
	2000: Greenwich University	



Figure 2: (above) Conference Poster

Figure 3: (below) Cardiff Castle, the conference banquet venue





CSMA Prizes:

for all inclusions under
CSMA
please contact:
Francisco Chinesta
francisco.chinesta
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Every year CSMA rewards the best two PhD thesis of the year. For the 2015 edition, the “CSMA prize comitee has examined 26 applications. The two awardees are Thanh Tung NGUYEN and Liang XIA. Liang XIA is designated as the CSMA candidate for the ECCOMAS award for the best Phd theses in 2015.

Thanh Tung NGUYEN: Modeling of complex microcracking in cement based materials by combining numerical simulations based on a phase-field method and experimental 3D imaging.

Advisors: Julien Yvonnet (MSME), M. Bornert, C. Chateau (laboratoire NAVIER).

Figure 1:
Thanh Tung NGUYEN



The goal of the PhD is to develop an approach combining numerical simulations and experimental techniques to model complex microcracking in heterogeneous cementitious materials. The proposed numerical model allows to predict accurately in 3D the initiation and the propagation of microcracks at the scale of the actual microstructure of a real sample subjected to compression. Its predictions have been validated by a direct comparison with the actual crack network characterized by 3D imaging techniques. The phase-field method is applied to microcracking simulations in highly heterogeneous microstructures and its advantages for such simulations are discussed. Then, the technique is extended to account for interfacial cracking, possibly occurring at inclusion/matrix interfaces. In a second part, the procedures to obtain the evolution of the 3D crack network within the samples by means of X-rays computed microtomography and in-situ mechanical testing are presented. The developed image processing tools based on digital volume correlation are used to extract with good accuracy the cracks from the grey level images. In a third part, are compared the predictions of the numerical model with experimental results obtained, first, with a model material made of expanded polystyrene beads embedded in a plaster matrix, and second, to a more complex lightweight concrete. The obtained direct comparisons of 3D microcrack networks and their evolutions demonstrate the very good predictive capability of the numerical model.

Current situation: Thanh Tung holds a CNRS postdoctoral fellow position at LaMCoS – INSA Lyon where he studies the behaviour of colonies of Environmentally Assisted short Cracks.

Liang XIA: Topology optimization of nonlinear multiscale structures.

Advisor: Piotr Breitkopf, Laboratoire Roberval, Université de Technologie de Compiègne.

Figure 2:
Liang XIA



The thesis is dedicated to simultaneous design of both macroscopic structure and microscopic materials. The author treats the material optimization process as a generalized nonlinear constitutive behavior, and therefore the nonlinear scale-interface equilibrium problem can be resolved naturally within the multiscale framework by the FE2 method. The proposed model enables to obtain optimal structures with spatially varying properties realized by the simultaneous design of microstructures. Note that the FE2 method is extremely expensive in terms of computing time and storage requirements. Liang Xia has thus developed an adaptive surrogate model, using snapshot Proper Orthogonal Decomposition (POD) and Diffuse Approximation to substitute the microscopic solutions. As for more severe material nonlinearity, he employed the potential-based Reduced Basis Model Order Reduction (pRB MOR) parallelized on Graphics Processing Units (GPUs) enabling the design of multiscale elastoviscoplastic structures in realistic computing times and with affordable memory requirements. Then, he has employed the reduced-order Numerically EXplicit Potentials (NEXP) for the representation of the generalized constitutive behavior. He has shown that this explicit NEXP approximation can well serve the simultaneous design purpose providing ultraresolution structures at a significantly reduced computational cost. Liang has finally proposed an automatic design framework for nonlinear highly heterogeneous structures of which the underlying material model is governed directly by the realistic microstructural geometry and the microscopic constitutive laws.

Current situation: Liang holds a postdoctoral position at MSME where he works on microcracking and transport in porous materials.

CSMA selected two PhD thesis for the ECCOMAS Olympiads 2016:

Jérémy BLEYER and Sondes METOUI were selected to represent CSMA at the 6th PhD ECCOMAS Olympiad held in Crete, Greece, June 5-10, 2016 in conjunction with the VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 2016).

Jérémy BLEYER: Numerical methods for the yield design of civil engineering structures.

Advisor: *Patrick de Buhan, Ecole des Ponts ParisTech.*

His work aims at developing efficient numerical tools for a more rational and less empirical assessment of civil engineering structures yield design. As opposed to traditional methodologies relying on combinations of elastic computations, safety coefficients and local checking of critical members, the yield design theory seems to be a very promising tool for a more rigorous evaluation of structural safety. Lower bound static and upper bound kinematic approaches of the yield design theory are performed numerically using dedicated finite elements for plates in bending and shells in membrane-bending interaction. Corresponding optimization problems are then solved using very efficient conic programming solvers. The proposed tools are also extended to the framework of periodic homogenization in yield design, which enables to tackle the case of strong material heterogeneities. Numerical procedures are specifically tailored to compute equivalent homogeneous strength criteria and to use them, in a second step, in a computation at the structural level. Finally, the potentialities of the yield design approach are illustrated on two complex engineering problems: the stability assessment of high-rise reinforced concrete panels in fire conditions and the computation of the Paris-Austerlitz railway station canopy.

Current situation: Jérémy holds a postdoctoral position at Computational Solid Mechanics Laboratory, Ecole Polytechnique Fédérale de Lausanne.

Sondes METOUI: Separated representations for the multiscale simulation of the mechanical behavior and damages of composite materials.

Advisors: *Ivan Jordanoff, Amine Ammar in collaboration with Etienne Prulière and Frédéric Dau, at Arts et Métiers ParisTech.*

In her dissertation, an approach based on the proper generalized decomposition (PGD) is proposed to simulate the interfacial delamination under quasi-static loading. This technique coupled with a cohesive zone model (CZM) allows a significant reduction of the computational costs. Three classical failure tests (DCB, ELS, and MMF) have been modeled using PGD and FEM as references. These two methods have been implemented in conjunction with CZM to represent delamination in different fracture modes (two pure modes and a mixed mode). Both 2D and 3D models were developed and analyzed. For all failure modes, a close agreement is found between PGD, FEM, and analytical solutions with a proper choice of the main model parameters (mesh density, interface stiffness and fracture toughness). The two methods have been compared with regard to the force versus displacement curves, the damage variable evolution, the interface separation evolution and the stress distributions. It shows that PGD can be used as an alternative to overcome the computational drawbacks of FEM such as the rapid increase in the number of degrees of freedom, the large computational time, and the storage limitation. PGD was found appropriate to capture physical phenomena, which occurs at the interface between layers. Finally, reduction of the number of interface elements was achieved owing to the new PGD-CZM discretization strategy, which minimizes modeling complexity. This strategy is used also for dynamical transient applications. Other types of damages, such as matrix cracking are considered. A computationally efficient approach is presented for predicting the impact response of cross-ply laminates under a low velocity impact. This was achieved using an implicit Newmark's integration scheme. A bilinear cohesive law was used to model the delamination and crack growth. A new multiscale separated representation method to compute the mechanical behavior of composite materials with periodic microstructure involves both the space coordinates of the microscopic scale as well as the space coordinates of the macroscopic scale. For coupling each subdomain, an efficient algorithm is proposed and validated in order to address the numerical challenges.

Current situation: Sondes is currently Postdoctoral fellow at National Center for Scientific Research (CNRS), Bordeaux. She works on numerical investigations on the dynamic behaviour of composite bonded joints under laser shock. ●

Figure 3:
Jérémy BLEYER



Figure 4:
Sondes METOUI



General Assembly Meeting and Special Symposium

The seventh assembly meeting of JSCES was held at Takeda Hall, the University of Tokyo, Japan, on May 27th, 2016 (Figure 1).

Both the operating and financial review for the previous fiscal year and operation and financial plan for this fiscal year were reported in this meeting. On this occasion, Prof. Kenjiro Terada (Tohoku University) was addressed as the new president of the JSCES. Prof. Takahiro Yamada (Yokohama National University) and Dr. Yasuyoshi Umezu (JSOL Corporation) were also addressed as the vice-presidents. The assembly

meeting was followed by a special symposium, in which a lecture was given by Prof. Masanori Kikuchi of Tokyo University of Science. He presented a talk entitled "Encouragement of experiments – the ongoing issues of crack propagation analysis -" (Figure 2).

Figure 2:
Prof. Masanori Kikuchi



Figure 1:
General assembly meeting



Award Ceremony for JSCES Prizes

On the same day, JSCES prizes were offered to senior and young researchers and practitioners. This year's recipients were: Prof. Kazuo Kashiya (The JSCES Achievements Award), Mr. Kazuto Yamamura (The JSCES Achievements Award), Dr. Hiroshi Watanabe (Kawai Medal), Dr. Hiroshi Akiba (Shoji Medal), Dr. Takashi Yamada (Technology Prize), and Mr. Koji Yamamoto (Technology Prize). Paper awards associated with the Transaction of the JSCES (see, <https://www.jstage.jst.go.jp/browse/jscs>) were also given to the following researchers: Profs. Junji Kato, Shinsuke Takase, Kenjiro Terada & Takashi Kyoya (Outstanding Paper Award), Prof. Susumu Shirayama (Outstanding Paper Award), Dr. Tomohiro Degawa (Young Researcher Paper Award),

Mr. Takeki Yamamoto (Young Researcher Paper Award). Also, a new award for young researchers who published an outstanding PhD thesis, was given to Dr. Yasunori Yusa (PhD Thesis Award). Moreover, Prof. Masaki Shiratori was awarded as an honorary member, and Prof. Kazuo Kashiya, Mr. Hiroshi Takahara and Dr. Akira Tezuka were awarded as fellow members (Figure 3).

Figure 3:
Group shot of the recipients of the JSCES Awards



Research Committee on Hyper-Complex Disaster Simulation (HCDS) in JSCES

Research Committee on Hyper-Complex Disaster Simulation (HCDS) in JSCES has been continuing intense research activities for frontal development of disaster simulations of Earthquake, Tsunami, Heavy rain and other natural disasters. The committee chairman is Prof. Kenjiro Terada, International Research Institute of Disaster Science (IRIDeS) at Tohoku University. The current members of HCDS consist of 20 academic researchers and 11 corporate researchers.

The main difficulties for natural disaster simulations are complex modeling of multi-physics behaviors and its large scaled computation in wide areas. Strong

Annual Conference

The 21st JSCES's Annual Conference on Computational Engineering and Science, chaired by Dr. H. Watanabe (MSC Co.), was held during May 31 – June 2, 2016, at Toki Messe Convention Center (Niigata, Japan). The conference was attended by about 450 participants, and over 310 papers with full lectures were presented by researchers, graduate students and practitioners. Fruitful discussions were exchanged in 30 organized sessions associated with a plenary lecture, a special event for young engineers, graphic awards and special symposia.

On the second day of the conference, a special lecture entitled "Application of numerical simulation in NAMICS Co." was given by Mr. T. Enomoto of NAMICS Co., a leading company of conductive and insulating materials for electronics. He presented how the company applied numerical simulations and experiments to develop a chipcoat such as Flip Chip Underfill, which is an insulating material used in mounting technologies involving direct electrical connections (Figure 4).



Figure 4:
Special lecture entitled
"Application of numerical
simulation in NAMICS Co"

The lecture was followed by a special panel discussion chaired by Prof. K. Terada. It was delivered by eight professors and researchers who represented each field in computational engineering and science, reflecting on the past 20 years and foreseeing the 20 years from now. At the former part of the session, Prof. T. Yamada stated the issues of stress analysis in solid and structural mechanics, Prof. K. Kashiwama reflected the advances in computational fluid mechanics, Prof. S. Hagiwara summarized the advances in meshfree methods and particle methods, and Prof. N. Takano talked on quality management of FEM analysis. At the latter part, Dr. R. Sawada introduced the history and the future of CAE application in industrial companies, Prof. M. Hori showed the play role of computational mechanics in earthquake disaster prevention, Prof. K. Nakajima made a survey of the field of supercomputing, and Prof. K. Ono forecasted the development of visualization techniques (Figure 5).



Figure 5:
Special panel discussion
chaired by Prof. K. Terada

After the panel discussion, an award ceremony for the new JSCES scholarship award, which was founded by the 20th Anniversary donation, was held. This year, the awards were presented to Mr. Takashi Kuraishi (Waseda Univ.), Mr. Yuto Soma (Ibaraki Univ.), and Mr. Gai Kubo (Univ. of Tsukuba) (Figure 6, Figure 7).



Figure 6:
Mr. Takashi Kuraishi



Figure 7:
Mr. Yuto Soma

nonlinearity and discontinuous behavior of solids are required for the discussion of failure process in structures, and complex fluid flow simulations in real geographical model should be implemented for flood disasters by introducing advanced turbulence models because of lack of resolution. Finally, fluid-structure interaction simulation is strongly desired in practical work for prevention/mitigation from several types of natural disasters. The aim of HCDS is to share our knowledge for modeling of hyper-complex behavior during natural disasters and to develop a frontal simulation framework for natural disasters (Figure 8).

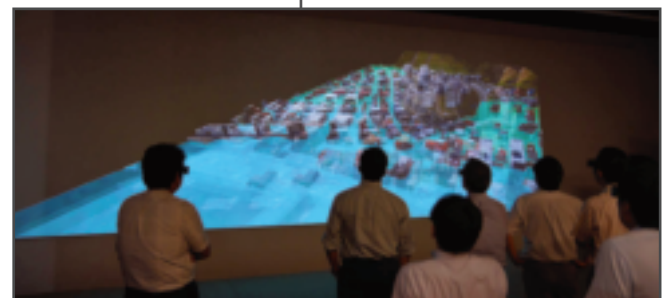


Figure 8:
Participants experiencing the virtual reality of
disaster simulations

For all inclusions under
JACM news

please contact:

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jacm-jim@save.sys.t.u-tokyo.ac.jp

The JACM is a union of researchers and engineers working in the field of computational mechanics mainly in Japan. JACM is 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>).

JACM participated the Fifth Computational Mechanics Symposium organized by the Science Council of Japan (SCJ), on December 7, 2015. 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 Minister, 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 annual SCJ Computational Mechanics Symposium has become a new tradition and is an evidence of how Japanese science and engineering community finds computational mechanics to be a very important area.

Figure 1:
Professor Genki Yagawa
(SCJ Member, Former
President of IACM) making
the opening remarks



In the fifth symposium, eight young researchers representing the participating computational mechanics related societies presented their latest research outcomes. From JACM Professor Akihiro Takezawa of Hiroshima University participated the symposium. He is the recipient of 2015 JACM Young Investigator Award. He presented the latest research outcomes of his research on the development of porous material using the computational mechanics approach and 3D printer.

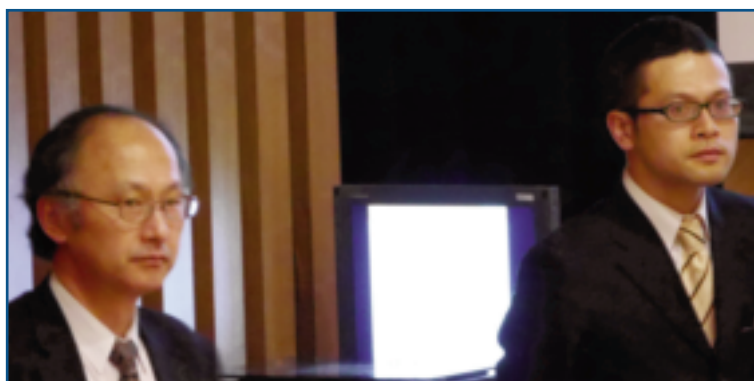


Figure 2:
Professors S. Yoshimura
(President of JACM) and
A. Takezawa (Hiroshima
University) in discussions
after the presentation by
Professor A. Takezawa

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)”.

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



Figures 3:
Professor I. Hagiwara making the
closing remarks

- Professor Mayuko Iwamoto (JSIAM, Meiji University) on adhesive locomotion in gastropods
- Professor Kazuki Niino (JASCOME, Kyoto University) on BEM analyses on electromagnetic scattering problems
- Professor Tomoaki Tatsukawa (CAE Konwakai, Tokyo University of Science) on multi-objective optimization of aeroacoustic problem using the K computer
- Dr. Takahiro Kikuchi (JSCES, Japanese Red Cross Musashino Hospital) on Hamilton MPS method with wall boundary conditions
- Professor Kaoru Iwamoto (JSME, Tokyo University of Agriculture and Technology) on direct numerical simulation for the reduction of friction drag in turbulent flow based on a biomimetic approach
- Professor Akihiro Takezawa (JACM, Hiroshima University) on the development of porous material using 3D printer and computational mechanics approach
- Professor Kohei Murotani (JSST, The University of Tokyo) on program library for the computations of particle method on parallel distributed memory computer and Tsunami simulation
- Dr. Daisuke Matsuoka (VSJ, Japan Agency for Marine–Earth Science and Technology) on the visualization of multivariable data and visualization analysis

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

Figures 4:
Organizers and speakers of computational mechanics symposium



JSME Certification Program of Computational Mechanics Engineer

JACM has collaborated the “Certification Program of Computational Mechanics Engineer “ of the Japan Society of Mechanical Engineer (JSME) (<http://www.jsme.or.jp/English/>)(<http://www.jsme.or.jp/cee/cmnnin-tei.htm>). The JSME has initiated the certification program in 2003. A number of computational mechanics-related societies in Japan have collaborated the program and JACM has been one of them. The purpose of this program is to qualify the levels of knowledge as well as skill of a computational mechanics engineer needed to independently perform reliable and accurate computational mechanics analyses. The scope of the certification program covers the starting to senior engineers, and spans the finite element method, the boundary element method, the finite difference method and other numerical analysis methods used in computational mechanics. This program has certified 6,800 computational mechanics engineers since 2003.

Since 2014, the highest level of the JSME certification “Senior Analyst Qualification” has been regarded to be equivalent to “Professional Simulation Engineer (PSE)” of NAFEMS, the International Association for the Engineering Analysis Community.



New Engineering Research Institute in Argentina

A new research center was created in Cordoba, Argentina, in October 2015: the Institute for Advanced Studies in Engineering and Technology (IDIT). The institute was created by agreement between the Argentinean National Council for Scientific and Technological Research (CONICET) and the National University of Cordoba (UNC). IDIT is hosted by the Faculty of Exact, Physical and Natural Sciences (FCEFyN) of UNC. Prof. Luis A. Godoy, a founding member of the Argentinean Association for Computational Mechanics (AMCA) has been appointed as the first director of IDIT.



Some forty people currently work at IDIT, including 17 researchers from CONICET and UNC, four post-docs, and doctoral students working under CONICET scholarships. All IDIT researchers provide support to the doctoral program in Engineering at FCEFyN by teaching doctoral courses and participating in the governance of the program. The group has gained strong recognition in Argentina from AMCA for their work in Computational Mechanics, and from IEEE in digital communications.

IDIT started as the confluence of five groups working independently at FCEFyN. The areas of research include computational modeling and testing for addressing problems of

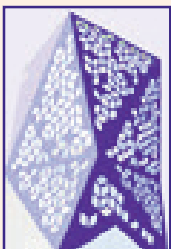
- Digital communication and information technologies. Research specializes on theory and technology of communications, emphasizing algorithms for signal processing for fiber-optic and wireless channels and data processing for networks.
- Mechanics of solids and structures. Modeling of nonlinear dynamics and buckling of structural systems, impact problems, Unsteady and nonlinear aero-servo-elasticity, metal forming processes, and new finite elements are performed with applications to understanding the behavior of wind turbine blades, wing flexibility, oil storage tanks, and non-destructive identification of concrete structures.
- Geomechanics and Geotechnologies. Research interests include soil and rock mechanics, foundations, dynamic properties of geo-materials, environmental geotechnics, flow through porous media, and subsurface water.

Figure 1:

IDIT researchers (from left to right)
Jorge Finochietto, Sergio Elaskar, Magalí Carro-Pérez, Graciela Corral-Briones, Marcelo García, Andrés Rodríguez, Federico Pinto, Marcelo Ceballos, Franco Francisca, Marcos Montoro, Damián Morero, Luis Godoy, Sergio Preidikman, Fernando Flores, Mario Hueda, Benjamín Reyes



Call for Papers



ENIEF 2016

XXII CONGRESS ON NUMERICAL METHODS AND THEIR APPLICATIONS
SYMPOSIUM IN HONOR OF PROF. LUIS A. GODOY

8 - 11 November 2016. Córdoba, Argentina

The Argentine Association for Computational Mechanics (AMCA) announces the XXII Congress on Numerical Methods and their Applications, ENIEF 2016.

As part of ENIEF 2016, a Symposium in honor of Prof. Luis A. Godoy, on the occasion of his 65th anniversary and in recognition of his academic and scientific achievements, will be held. The main objective is to bring together colleagues and disciples of Professor Godoy to pay him a deserved tribute.

The congress will be organized by the National Technological University, Córdoba's Regional Faculty (Facultad

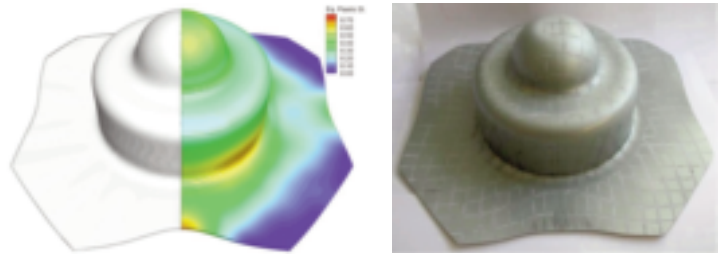


Figure 2:

The figure compares the final shapes obtained experimentally and with numerical simulation of an industrial multi-step deep drawing process. The equivalent plastic strain is plotted over the deformed shape of the simulation (work done by Fernando Flores based on in-house software)

- Hydraulics and Hydrology. Research covers limnology, river, and marine environments using advanced computational methods. Detailed studies to design of hydraulic infrastructure complemented with modern experimental facilities are also developed. The group hosts a modern meteorological radar, the first developed in Argentina.
- Mechanics of aerospace fluids. Lines of research include modeling of supersonic flow, chemically active flow (for simulating explosions and re-entry of vehicles to the atmosphere), magneto-gas-dynamics (for plasma propulsion), and chaotic intermittence.

Efforts have been made over the last two years to generate synergic activities between groups in order to foster new interdisciplinary research. These include new ideas focusing on

- Vulnerability of infrastructure and environment associated with the storage and transport of hydrocarbon fluids, and
- Digital remote sensor processing for meteorological and natural events affecting societal and environmental safety.

Strong collaboration has been developed over the years by IDIT researchers with other research institutions abroad in the form of joint projects and research exchanges, notably with Spain (Polytechnic University of Cataluña, Polytechnic University of Madrid, Universidad Autónoma de Madrid, Carlos III University of Madrid), United States (United States Geological Survey, West Virginia University, Virginia Tech, University of North Carolina at Charlotte, University of Puerto Rico, University of Maryland, University of Illinois at Urbana-Champaign), Italy (Polytechnic of Torino), France (Unité de Recherche Hydrologie-Hydraulique), and Finland (Aalto University).

Contact: idit@fcefyn.unc.edu.ar, & <http://www.inv.idit.efn.uncor.edu/> ●

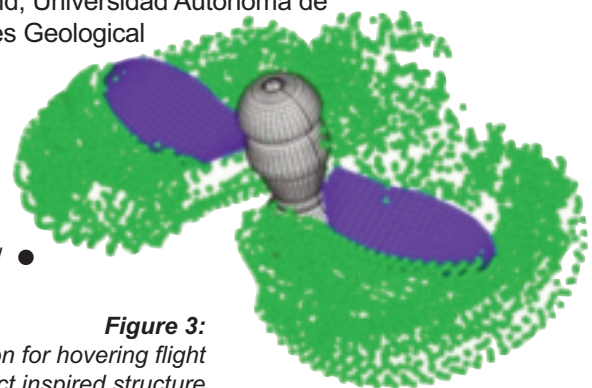


Figure 3:

The figure shows the three-dimensional wake visualization for hovering flight combined with flapping motion of an insect inspired structure (work done by Sergio Preidikman and Bruno Rocca based on in-house software)

Regional Córdoba) and will take place in Córdoba, Argentina.

Córdoba, also referred to as La Docta, is one of the most populous Argentinian city after Buenos Aires. Located in the central part of Argentina, Córdoba is an important tourist, cultural, economic and educational center of the region. With the presence of many universities and research centers, it is home of a large number of university students from all the country and the world.

We look forward to your valuable participation in this important event. We will be waiting for you.

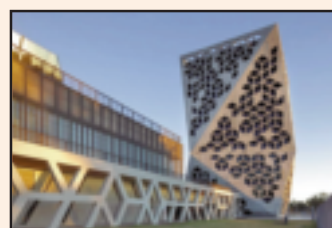
Deadline for abstract submissions: **21 May 2016**

e-mail: enief2016@frc.utn.edu.ar

Web: www.frc.utn.edu.ar/enief2016/ ●

Figure 2:

Prof. Luis A. Godoy



The German Association for Computational Mechanics
(GACM)
celebrates its 25th Anniversary

on the occasion of the ECCOMAS Congress 2016

Some Snapshots from 25 Years of GACM History:



Figure 1:
GACM Honorary Presidents, from left to right:
Professor Walter Wunderlich (GACM President 1990-2000),
Professor Erwin Stein (GACM Vice President 1990-2000)
Professor Ekkehard Ramm (GACM President 2000-2008)

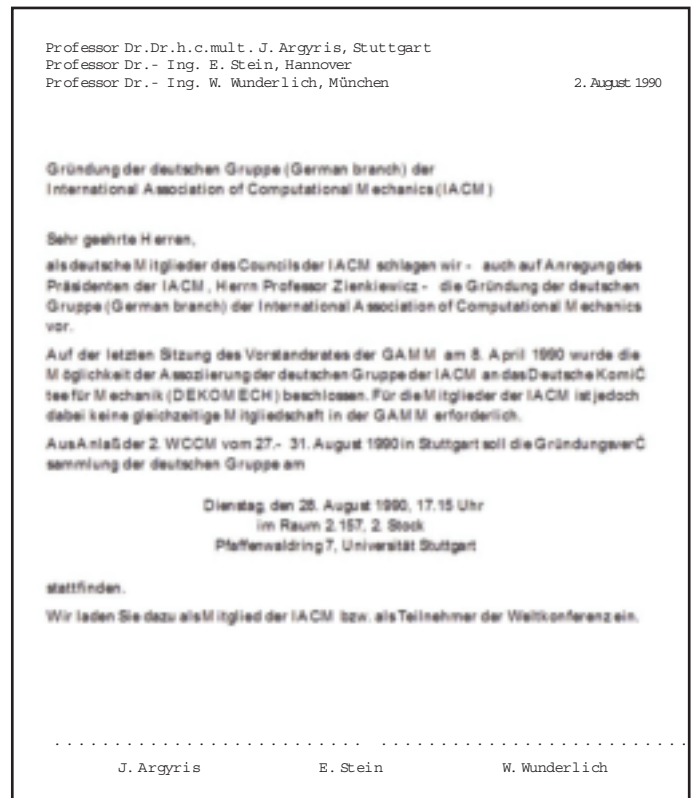


Figure 2:
The original invitation letter for the founding meeting of GACM as German branch of the International Association for Computational Mechanics (IACM), which took place at the University of Stuttgart in August 1990. The initiators were Professor John Argyris, Professor Erwin Stein and Professor Walter Wunderlich

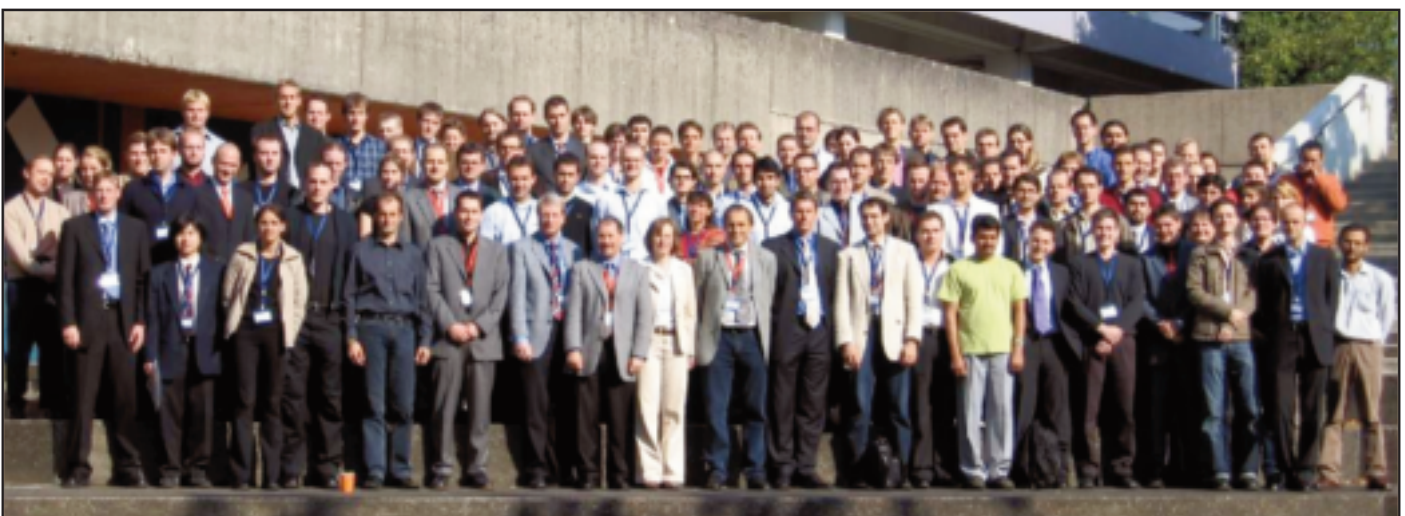


Figure 3:
The participants of the 1st GACM Colloquium on Computational Mechanics at the Ruhr-University Bochum in 2005, which marked the beginning of a successful and long-standing GACM tradition (with further colloquia being organized in Munich 2007, Hannover 2009, Dresden 2011, Hamburg 2013 and Aachen 2015). The 7th GACM Colloquium will be hosted by the University of Stuttgart in 2017

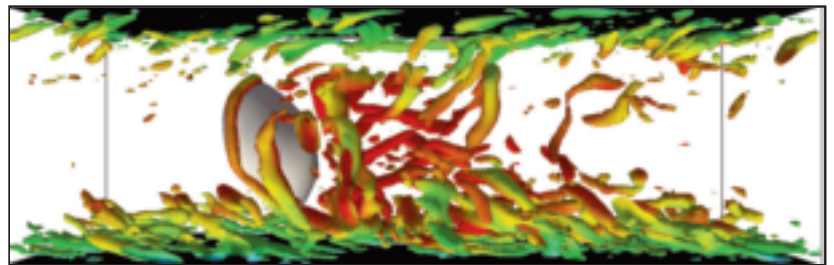
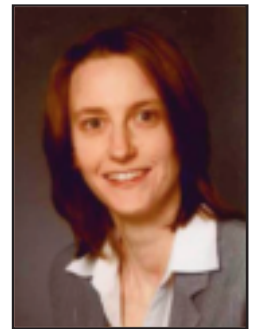
GACM Best PhD Awards

In 2012, GACM has successfully established an award for young academics, namely the GACM Best PhD Award. It is our great pleasure to announce that not only one but two outstanding doctoral theses will be honored with this award for the year 2015. The awardees are **Dr.-Ing. Ursula Rasthofer** for her thesis "**Computational Multiscale Methods for Turbulent Single and Two-Phase Flows**" and **Dr.-Ing. Richard Ostwald** for his thesis "**Modelling and Simulation of Phase-Transformations in Elasto-Plastic Polycrystals**".

Dr. Rasthofer's work led to a doctoral degree from the Technical University of Munich (TUM) and has been performed under the academic supervision of Dr. Volker Gravemeier. Dr. Ostwald conducted his work at the Technical University of Dortmund under the academic supervision of Prof. Andreas Menzel. The two awards will be officially conferred at the next GACM Colloquium in Stuttgart in 2017.

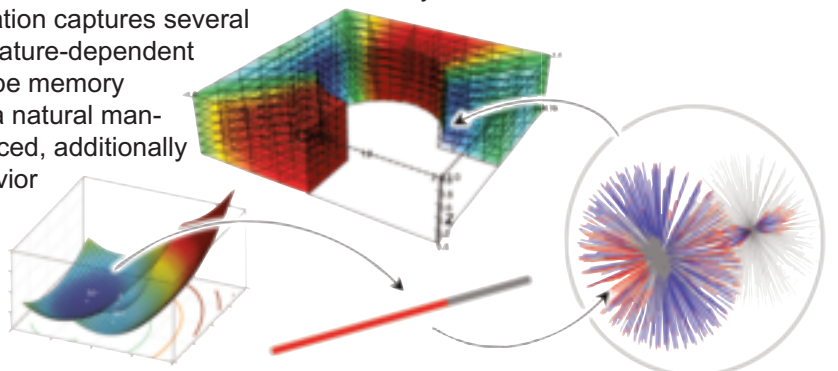
"Computational Multiscale Methods for Turbulent Single and Two-Phase Flows" (Dr.-Ing. Ursula Rasthofer)

In the first part of the thesis, large-eddy simulation of turbulent single-phase incompressible flow is considered. Therefore, an approach is built up from the framework of the variational multiscale method. The derived approach incorporates multifractal subgrid-scale modeling with scale separation by level-transfer operators from plain aggregation algebraic multigrid methods. Further steps address its extension to passive-scalar mixing and weakly compressible flow. For two-phase flow, examined in the second part, a face-oriented stabilized Nitsche-type extended finite element method is introduced. The proposed method makes use of a level-set description for the interface and jump enrichments to capture the related discontinuities in the flow field. Independent of the interface position, stability is ensured for the entire range from viscous-dominated laminar to highly transient turbulent flow. The two individual methods are eventually unified, leading to a novel and comprehensive approach to large-eddy simulation of turbulent two-phase flow.



"Modelling and Simulation of Phase-Transformations in Elasto-Plastic Polycrystals" (Dr.-Ing. Richard Ostwald)

In his thesis, Dr. Ostwald introduces a new framework for the simulation of shape memory alloys (SMA) and TRIP steels undergoing martensite-austenite phase-transformations. The goal of the work is the derivation and elaboration of a generalized model which facilitates the reflection of the characteristic macroscopic behavior of SMA as well as of TRIP steels. The foundation of the overall formulation is a scalar-valued, thermodynamically consistent, statistical physics based model for the simulation of phase-transformations in solids. As the work proceeds, the model is implemented in affine and non-affine micro-sphere formulations in order to capture polycrystalline behavior and to simulate three-dimensional boundary value problems. It is shown that the proposed formulation captures several experimentally observed effects such as temperature-dependent pseudo-elasticity and pseudo-plasticity, the shape memory effect itself, and polycrystalline grain-locking in a natural manner. Moreover, a coupling to plasticity is introduced, additionally enabling the capturing of the macroscopic behavior of TRIP steels. Finally, the implementation of a three-dimensional finite-deformation phase-transformation model that focuses on representative transformation directions is elaborated in a thermo-elastoplastic framework. ●



IUTAM Symposium on Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions



Figure 1:
USACM President Somnath Ghosh speaking at the USNCCM13 banquet in San Diego in July 2015

The *IUTAM Symposium on Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions* will be held in the Inner Harbor of Baltimore, USA, on June 20-22, 2016. It is organized by Prof. Somnath Ghosh, current USACM President and M. G. Callas Professor at Johns Hopkins University. Hosted by Johns Hopkins University, this symposium is sponsored by US Association of Computational Mechanics with support of U.S. National Committee on Theoretical and Applied Mechanics (USNC/TAM). It is bringing together experts in Computational and Experimental Mechanics, and Materials Science to discuss multidisciplinary approaches in integrated modeling and simulation, characterization and experiments to predict extreme deformation and failure in heterogeneous materials. The conference is being financially co-sponsored by National Science Foundation, Army Research Office and Los Alamos National Laboratory. It will have 35 keynote lectures, 20 posters by junior researchers and 3 industry led panels on future research directions.

Celebration of Professor Ivo Babuska's 90th Birthday

Advances in Mathematics of Finite Elements (AMFE 2016) was held at the Institute for Computational Mechanics in Austin, Texas, March 21-22, 2016. The purpose of this two day workshop was to bring together leading researchers in the field of mathematics of finite elements. Organized by Leszek Demkowicz (UT-Austin), Richard Falk (Rutgers University), Benqi Guo (University of Manitoba), Zhimin Zhang (Beijing Computational Science Research Center and Wayne State University), and Michael Vogelius (Rutgers University), the workshop was also held in honor of the 90th birthday of Professor Ivo Babuska.

The following twelve speakers made presentations during the two-day workshop: Douglas Arnold (University of Minnesota), Uday Banerjee (Syracuse University), Susanne Brenner (Louisiana State University), Benqi Guo (University of Manitoba), Robert P. Lipton (Louisiana State University), Jens Markus Melenk (Vienna University of Technology), J. Tinsley Oden (ICES, UT-Austin), Christoph Schwab (ETH), Manil Suri (University of Maryland Baltimore County), Barna Szabo (Washington University), Michael Vogelius (Rutgers University), and Zhimin Zhang (Beijing Computational Science Research Center and Wayne State University). In addition, there were 29 posters presented from leaders in the area of finite elements.

Figure 2:
AMFE 2016 Workshop Participants



A workshop dinner was held on the last evening at the University of Texas Alumni Center. During this time, Professor Babuska's many contributions to mathematics and his influences on the lives of his students and colleagues were celebrated. To read more about the workshop and view photos and

recordings of the oral presentations, go to <http://www.amfe2016.usacm.org>. An article on this event also appeared in the New York Times: http://www.nytimes.com/2016/04/25/opinion/the-mathematicians-90th-birthday-party.html?_r=0

USACM Upcoming Events

- **IUTAM Symposium on Integrated Computational Structure-Material Modeling of Deformation and Failure Under Extreme Conditions**, Baltimore, MD, June 20-22, 2016, iutam2016ics.usacm.org.
- **Advances in Computational Methods for Nanoscale Phenomena**, Ann Arbor, MI, August 29-31, 2016, acm-nano.usacm.org
- **Analysis and Meshfree Methods**, La Jolla, CA, October 10-12, 2016, iga-mf.usacm.org
- **U.S. National Congress on Computational Mechanics (USNCCM14)**, July 17-20, 2017, Montreal, Canada, 14.usnccm.org ●

Workshop on Multiscale Methods and Validation in Medicine and Biology III

The *Workshop for Multiscale Methods and Validation in Medicine and Biology III* was held February 25-26, 2016 on the University of California, Los Angeles campus. The workshop was organized by Bill Klug (UC-Los Angeles), Ellen Kuhl (Stanford), Alex Levine (UC-Los Angeles), Christoph Haselwandter (USC), Krishna Garikipati (University of Michigan) and Tarek Zohdi (UC-Berkeley) and was the third meeting in the series. It brought experimental and computational researchers together in a forum to discuss the challenges of predictive modeling and validation for biomechanics and mechanobiology across scales. There were 23 talks and 10 poster presentations with ample time for discussions. The participants also enjoyed a dinner at the historic Skylight Gardens near the campus.



Figure 3:
*Poster session participants
at MMVMB workshop*

Workshop on Nonlocal Models in Mathematics, Computation, Science, and Engineering

The *Workshop on Nonlocal Models in Mathematics, Computation, Science, and Engineering* was held at Oak Ridge, Tennessee, October 26-28, 2015. The 3-day workshop was organized by Pablo Seleson (Oak Ridge National Laboratory), Clayton Webster (ORNL), Michael Parks (Sandia National Laboratories) and Tadele Mengesha (University of Tennessee, Knoxville). Featuring 25 talks and 2 poster sessions and attended by over 50 researchers, the workshop achieved its purpose of bringing together experts from the mathematical, computational, scientific, and engineering communities who work with nonlocal models and provide a platform for the exchange of ideas. Visit <http://www.nlmcse.usacm.org> to download abstracts and read more about the event.



Figure 4:
*Participants at Nonlocal
Models Workshop in Oak
Ridge, Tennessee*

Election of New Executive Committee Members

In April, current President, Somnath Ghosh (Johns Hopkins University) announced the results of USACM election for the new Secretary/Treasurer and Members-at-Large. The results were as follows:

Secretary/ Treasurer: **Yuri Bazilevs** (University of California, San Diego)

Members-at-Large: **Ellen Kuhl** (Stanford University), **Shaofan Li** (University of California, Berkeley), **Alison Marsden** (Stanford University), and **Jessica Zhang** (Carnegie Mellon University).

Their terms will begin immediately at the end of July, 2016. ●

conference diary planner

11 - 14 July 2016	ICCMS2016 : VI Int. Congress on Computational Mechanics and Simulation		
<i>Venue:</i>	Bologna, Italy	<i>Contact:</i>	http://conference.mercatura.pt/mechcomp2016/
24 - 29 July 2016	APCOM 2016: 6th Asia Pacific Congress on Computational Mechanics		
<i>Venue:</i>	Seoul, Korea	<i>Contact:</i>	http://apacm-association.org
24 - 29 July 2016	WCCM XII: World Congress on Computational Mechanics		
<i>Venue:</i>	Seoul, Korea	<i>Contact:</i>	http://www.wccm-apcom2016.org/
21 - 26 Aug 2016	24th International Congress of Theoretical and Applied Mechanics		
<i>Venue:</i>	Montreal, Canada	<i>Contact:</i>	http://www.ictam2016.org/
21 - 23 Sept. 2016	MMHS 2016 - Multiscale Modeling of Hetrogeneous Structures		
<i>Venue:</i>	Dubrovnik, Croatia	<i>Contact:</i>	http://www.ceacm.org/
10 - 12 Oct. 2016	Analysis and Meshfree Methods		
<i>Venue:</i>	La Jolla, CA, U.S.A.	<i>Contact:</i>	http://iga-mf.usacm.org/
6 - 9 Nov. 2016	CILAMCE 2016 - Iberian-Latin-American Congress on Computational Methods in Engineering		
<i>Venue:</i>	Brasilia, DF, Brasil.	<i>Contact:</i>	http://2016.cilamce.com.br/
8 - 11 Nov. 2016	ENIEF 2016 - XXII Congress on Numerical Methods and their Applications		
<i>Venue:</i>	Córdoba, Argentina	<i>Contact:</i>	http://www.frc.utn.edu.ar/enief2016/
6 - 7 April 2017	SYMCOMP 2017 - Int. Conf. Numerical & Symbolic Computation: Developments & Applications		
<i>Venue:</i>	Minho, Portugal	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
15 - 17 May 2017	VII International Conference on Computational Methods in Marine Engineering		
<i>Venue:</i>	Nantes, France	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
15 - 17 May 2017	MultiBioMe 2017 - Multiscale Problems in Biomechanics and Mechanobiology		
<i>Venue:</i>	Corsica, France	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
6 - 9 June 2017	SMART 2017 - 8th Conference on Smart Structures and Materials		
<i>Venue:</i>	Madrid, Spain	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017/
12 - 14 June 2017	COUPLED PROBLEMS 2017 - VII Int. Conf. on Coupled Problems in Science & Engineering		
<i>Venue:</i>	Rhodes Island, Greece	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
14 - 16 June 2017	CFRAC 2017 -V Int. Conf. Computational Modeling of Fracture & Failure of Materials & Structures		
<i>Venue:</i>	Nantes, France	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
19 - 21 June 2017	X-DMS 2017 - eXtended Discretization Methods		
<i>Venue:</i>	Umeå University, Sweden	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
26 - 28 June 2017	ADMOS 2017 - VIII International Conference on Adaptive Modeling and Simulation		
<i>Venue:</i>	Lombardy, Italy	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
30 June - 1 July 2017	MDA 2016 - 1st International Conference on Materials Design and Applications 2016		
<i>Venue:</i>	Porto, Portugal	<i>Contact:</i>	www.fe.up.pt/mda2016
3 - 5 July 2017	CMN 2017 - Congreso de Métodos Numéricos en Ingeniería		
<i>Venue:</i>	Valencia, España	<i>Contact:</i>	http://congress.cimne.com/CMN2017/
11 - 14 July 2017	2nd Int. Conference Mechanics of Composites		
<i>Venue:</i>	Bologna, Italy	<i>Contact:</i>	https://sites.google.com/a/gcloud.fe.up.pt/mechcomp2016/
17 - 21 July 2017	USNCCM14 - 14th U.S. National Congress on Computational Mechanics		
<i>Venue:</i>	Montreal, Canada	<i>Contact:</i>	http://14.usnccm.org/
21 - 23 Aug. 2017	Modern Finite Element Technologies - Mathematical and Mechanical Aspects		
<i>Venue:</i>	Bad Honnef, Germany	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
5 - 7 Sept. 2017	COMPLAS 2017 - XIV International Conference on Computational Plasticity		
<i>Venue:</i>	Barcelona, Spain	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
13 - 16 Sept 2017	CMM-2017 - 22nd International Conference on Computer Methods in Mechanics		
<i>Venue:</i>	Lublin, Poland	<i>Contact:</i>	http://cmm2017.pollub.pl/
28- 28 Sept. 2017	PARTICLES 2017 - V International Conference on Particle-based Methods		
<i>Venue:</i>	Hannover, Germany	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017
11 - 13 Oct 2017	11th SSTA - 11th International Conference "Shell Structures: Theory and Applications"		
<i>Venue:</i>	Gdańsk, Poland	<i>Contact:</i>	http://www.ssta.pg.gda.pl
11 - 15 June 2018	ECCM - ECFD Conference 2018		
<i>Venue:</i>	Glasgow, UK	<i>Contact:</i>	http://www.eccomas.org/vpage/1/14/2017