

iacm expressions

**XFEM Simulation on Strong
& Weak Arbitrary
Discontinuity**

Z. Zhuang, Z. Liu & Q.Zeng

**Bridging Scales and
Mathematical Models with
a Generalized Finite
Element Method**

C. Armando Duarte

**Multiscale Modeling of
Plasticity in Amorphous
& Polymeric Materials**

S. Li, S. Urata
& T. Murashima

**Digital & Hybrid Twins:
When Data Meets Physics**

F.Chinesta, E. Cueto
& J.-L. Duval

**Reduced Basis Methods for
Partial Differential
Equations**

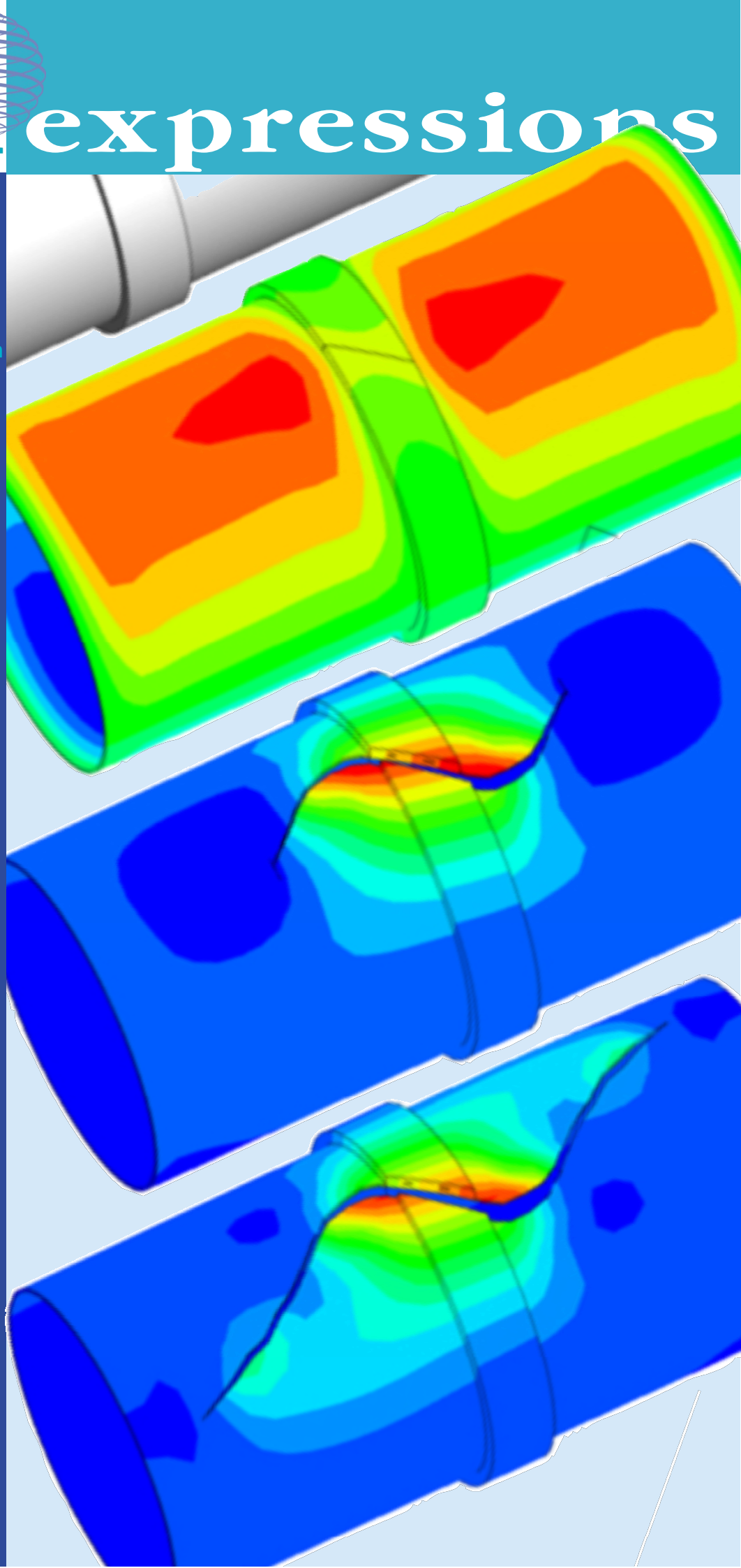
Book Report by Dan Givoli

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2	XFEM Simulation on Strong & Weak Arbitrary Discontinuity	Zhuo Zhuang, Zhanli Liu & Qinglei Zeng
6	Bridging Scales and Mathematical Models with a Generalized Finite Element Method	Carlos Armando Duarte
10	Multiscale Modeling of Plasticity in Amorphous & Polymeric Materials	Shaofan Li, Shingo Urata & Takahiro Murashima
14	Digital & Hybrid Twins: When Data Meets Physics. A new paradigm for simulation-based engineering	Francisco Chinesta, Elias Cueto & Jean-Louis Duval
20	Reduced Basis Methods for Partial Differential Equations by Alfio Quarteroni, Andrea Manzoni	Book Review by Dan Givoli
23	APMTAC	Portugal3
24	GACM	Germany6
27	JACM	Japan
28	JSCES	Japan 9
30	GIMC	Italy
31	KSCM	Korea
32	IACMM	Israel
34	UKACM	U.K.
36	CSMA	France
38	USACM	U.S.A.
40	SEMNI	Spain
42	PACM	Poland
44	AMCA	Argentina
46	Conference Diary Planner	

contents

The first issue of IACM Expressions was released on summer 1996. Over the last 23 years the pages of this magazine have witnessed the many advances in the broad field of computational mechanics and the continuous evolution and growth of the International Association for Computational Mechanics (IACM).

These facts are supported by figures. IACM is nowadays a prestigious international organization grouping 31 affiliated scientific associations from the five continents with some 5000 individual members who regularly participate in the many activities that IACM organizes and supports. These include the World Congress on Computational Mechanics (WCCM) that rotates biannually around the world (the next one will be held in Paris, France on 19-24 July 2020) and many specialized international scientific conferences on topics such as finite element in fluids, computational plasticity, coupled problems and adaptive modelling, just to name a few.

In the same period IACM has improved its organizational structure. The two main decision bodies are the Executive Committee (EC) and the General Council that are renewed periodically in a democratic form with participation of the IACM affiliated associations and its members. The main IACM officers in the EC are the President, the three Vice-presidents, representing all the world regions, and the General Secretary. During the life of this magazine the IACM bodies have been renewed many times. For instance, the IACM presidents in that period have been Alf Samuelsson (1995-1999), Thomas JR Hughes (1999-2002), myself (2002-2012); Genki Yagawa (2012-2015), Win Kam Liu (2015-2018) and Antonio Huerta, the current IACM president. Prior to that date IACM was pushed by two extraordinary presidents, Olgierd C. Zienkiewicz, the founder of the IACM in 1981, and Tinsley Oden. Profs. Zienkiewicz and Samuelsson are not longer with us and it is of justice to recognize the extraordinary work they did for giving shape and strength to the IACM in its early years, including the support for creating IACM Expressions.

The research fields of interest to the IACM community have also evolved over the past two decades. Indeed, classical topics such as development of constitutive models for new materials, or the search for numerical methods with enhanced accuracy are still the focus of many researchers. However, new research areas have emerged due to the need for solving larger and more complex problems in engineering and applied sciences. Some new keywords for current research on computational mechanics are multi-scale modelling of multidisciplinary problems, high performance computing, soft computing procedures based in artificial intelligence

and machine learning techniques, data-driven computing, digital twins and the computational design of new functional materials, among many others. The pages of this issue of IACM Expressions are an example of the diversity of current research in our community. The application range of computational methods has also widened to reach all fields of engineering and sciences, including medicine, biology and chemistry to name just a few broad disciplines where computational mechanics is meant to have a big impact.

The incorporation of efficient software within devices for a range of applications and the emergence of software-as-a service procedures that allow users to connect to and use cloud-based applications over the Internet, are opening new paradigms for taking the outputs of research in computational mechanics beyond the frontiers of standard common practice. The limits of application of the research in the computational mechanics field, therefore, seem to be expanding continuously.

As mentioned above, the pages of IACM Expressions have captured glimpses of this extraordinary story over the years. In addition, this magazine has tried to bring the good moments of the corporate life of the IACM closer to its members in an informal manner. Pursuing and extending these objectives for IACM Expressions in the next coming years will surely help the computational mechanics community to learn about new scientific and technical developments, as well as to follow up the successful evolution of the activities of the IACM and its members.

With these lines I would like to say good-bye to the readers of IACM Expressions, as in 2020 I will stop being the editor of this magazine. It has been a privilege to have had the opportunity to pilot the editorial line of the magazine for over two decades. I would like to express my gratitude to the IACM for the continuous support to my editorial activities, and to the IACM officers and staff who have supported the edition and publication of IACM Expressions since 1996. Special thanks go to Ms. Diane Duffett who has been the soul of this magazine and the responsible for its lay-out and timely publication for many years. My final thanks go to all who have contributed to the content of IACM Expressions over the years.

Long life and best of luck to IACM Expressions !

Eugenio Oñate
Editor of IACM Expressions
Past President of IACM

XFEM Simulation on Strong & Weak Arbitrary Discontinuity

by

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Introduction of strong and weak discontinuity

The extended finite element method (XFEM) formulation is developed for modeling of strong and weak arbitrary discontinuity. The conventional strong discontinuity is a fracture, which uses C^{-1} function described. An example is plotted in *Figure 1* with Mode I and Mode II hybrid crack propagation at 70° experimented by Kalthoff (1988) and crack growth at 72° simulated by our model.

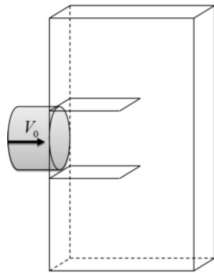
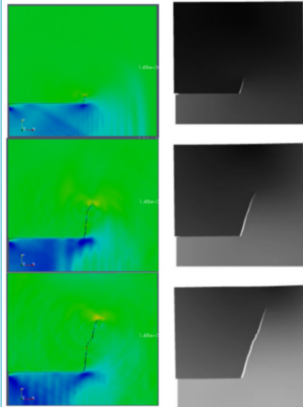


Figure 1:
Kalthoff crack
propagation by
experiment and XFEM
simulation



In contrast, the common weak discontinuity occurs on the interface of materials, crystal and phase boundaries. The particle/matrix composite interface at $f=0$ is plotted in *Figure 2*, which is a strain discontinuity in displacement field used C^0 function described.

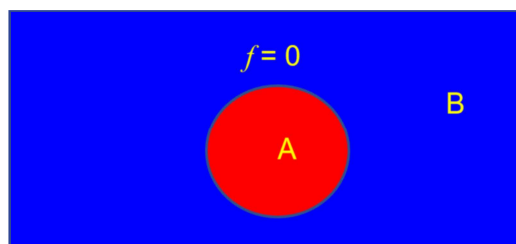
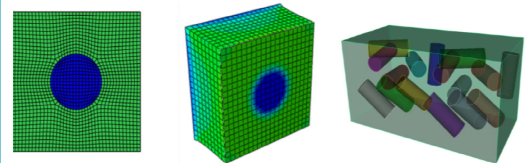


Figure 2:
Particle/matrix composite
with strain discontinuity
at interface

Distance to interface $f(x)$
 $f < 0$ located in phase A
 $f = 0$ located at interface
 $f > 0$ located in phase B

The level set function is used to evaluate the location of different phases. The advantage of XFEM is to adopt regular mesh and no need remeshing during material deformation, as illustrated in *Figure 3*. Another advantage of XFEM compared with FEM is no very small element close to interface to match the configuration.



FEM mesh

XFEM mesh

XFEM displacement field formula:

$$\begin{aligned} \mathbf{u}^h(x, t) &= \mathbf{u}^{\text{cont}}(x, t) + \mathbf{u}^{\text{enr}}(x, t) \\ &= \sum_{I \in S_{\text{cont}}} N_I(x) \mathbf{u}_I(t) + \sum_{J \in S_{\text{interface}}} N_J(x) \Phi(x) \mathbf{a}_J \end{aligned}$$

continuous discontinuous

Figure 3:
A particle/matrix composite
used by FEM and XFEM mesh,
as well as displacement field
formula

Strong discontinuity of continuum-based shell element

The shell structure is adopted here to express strong discontinuity, which has been widely used in the engineering, such as aircraft fuselages, ship hulls, pipelines and so on. Accurate prediction of crack initiation and propagation path in shell is of great importance to guarantee the safety and evaluate the failure of structure. FEM is a powerful tool to analyze the safety of shell structure. However, when coming to crack propagation problem, the classical FEM suffers from enormous work in remeshing.

XFEM is introduced into continuum-based (CB) shell element and both jump and crack tip enrichment functions are considered [1,2]. This method is improved to model stationary and propagating crack in shells [3]. In 1980s, the kinematics and constitutive equations are derived for “degenerated shell element” from 3D element based on Mindlin-Reissner assumptions. The model has been extended to nonlinear analysis[4].

In this study, a formulation of XFEM on CB shell element is proposed to model crack in shell structure, which can deal with geometrical nonlinearity simultaneously. The CB shell element is degenerated from 3D solid element. The crack is not necessarily perpendicular to the shell middle surface and slanted crack can be considered in CB shell element.

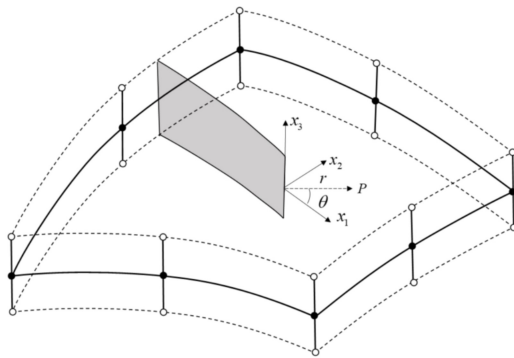


Figure 4:
A CB shell element containing a crack front

A quadratic CB shell element is depicted in Figure 4, which is composed of 8 master nodes and 16 slave nodes, denoted by filled nodes and empty nodes, respectively. Every two slave nodes are connected with one master node by a director, which can also be called as “fiber”. The nodal coordinates co-rotate with the fiber. The well-known Euler’s equations of motion can be solved at middle surface based on the master nodes.

The displacement approximation is based on the slave nodes. Both slave nodes and master nodes are enriched and the enrichment functions are established on slave nodes, as shown in Figure 5. For a CB shell element containing a crack front, the slave nodes are enriched by crack tip functions for 3D cracks. For the cracked elements behind the tip location, a Heaviside step functions are used for enrichment.

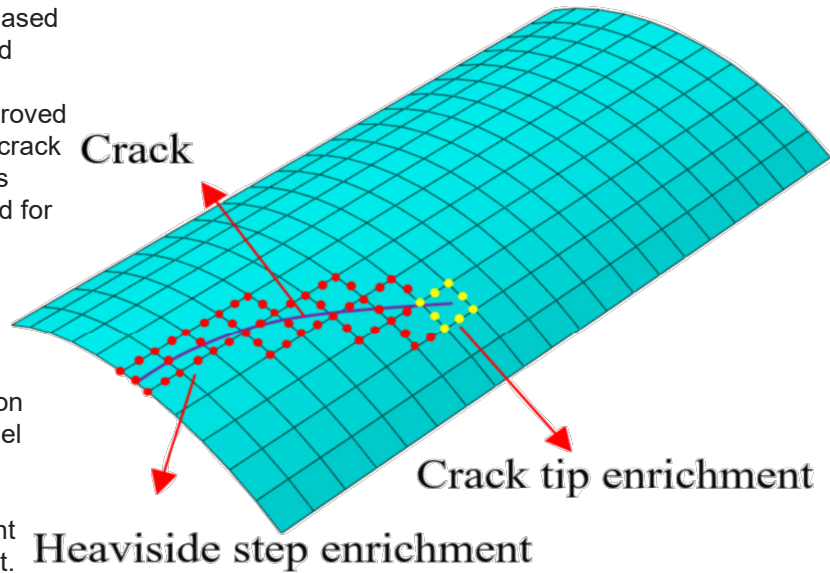
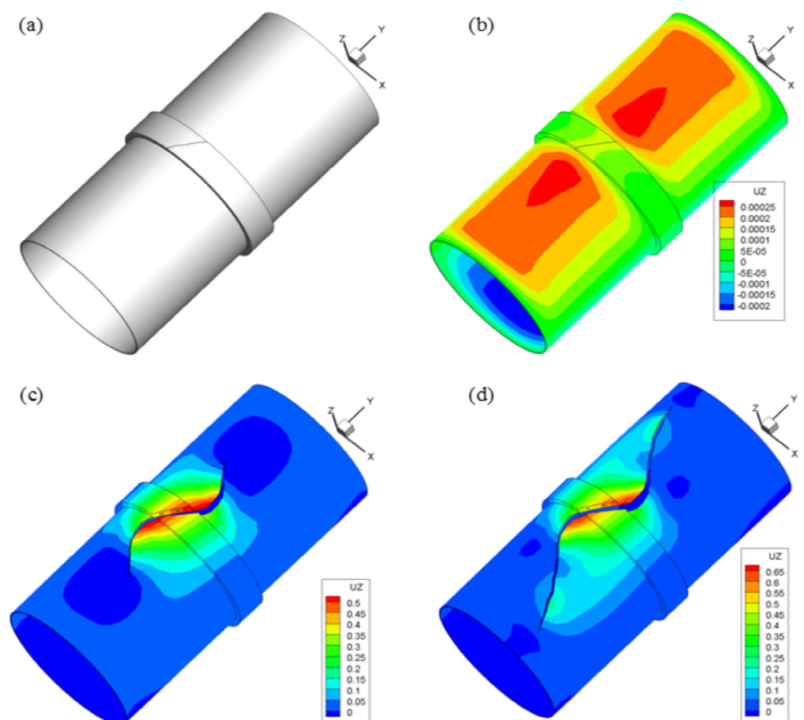


Figure 5:
XFEM enrichment of CB shell

An example of XFEM simulation on CB shell is the pressured pipeline with an inclined initial crack penetrated through thickness to a hoop band, as shown in Figure 6(a). The crack propagation path is shown in Figure 6(b~d). The crack propagates as a “wing crack” simulated by CB shell elements independent of the mesh. The XFEM technology is developed and implemented in CB shell element to model arbitrary crack propagation. Specially, the crack is not necessarily perpendicular to the middle surface of shell element and geometrical nonlinearity is considered. It should be pointed out that this method can be extended to elastic-plastic problems.

Figure 6:
Shell structure with inclined crack:
(a) geometry, (b~d) contour of displacement field in Z direction with internal pressure as 0.1MPa, 3.5MPa and 6.0MPa, respectively



T_{ref} (K)	A	B(K)	C_v (Jmm ⁻³ K ⁻¹)	n	K (GPa)	G_0 (GPa)	ρ (g/cm ³)
273	-10	107.54	1.977×10^{-3}	4	5.205	1.4818	1.18
p_1	p_2	p_3	p_4	q_1	q_2	q_3	q_4
0.0738	0.1470	0.3134	0.3786	463.4	0.06407	0.0001163	7.321×10^{-7}

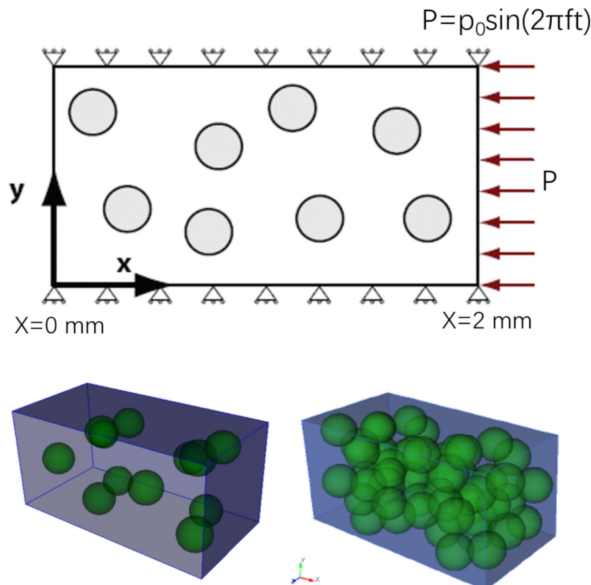
Table 1:
Parameters of matrix

The CB shell element is degenerated from 3D solid element and so many features are constructed based on solid element. For example, enrichment shape functions are calculated on solid element and 3D constitutive law can be used just with a little modification, as well as the level set method is adopted for 3D crack. The stress intensity factor is also calculated by equivalent domain integral method and interaction integral for 3D crack. However, it is found that the auxiliary fields with the leading terms for crack in Mindlin-Reissner plate can't satisfy exactly the equilibrium equations or the strain-displacement relationship, a revised term is retained in this study to get results independent of integral domain.

Weak discontinuity of polymer composite under shock wave

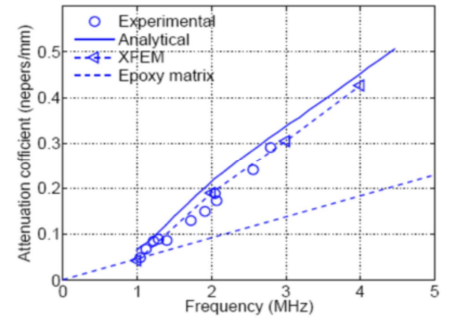
For the weak discontinuity by XFEM, an example is given to model the supersonic wave propagation in glass spheres/epoxy [5,6]. The model geometry configuration is 1x1x2mm with 40x40x80 brick elements. The shock wave period is $t_0=10^3\mu s$ with time increment is $\Delta t=1\mu s$. The glass spheres are randomly distributed in epoxy matrix by using random sequential adsorption (RSA) algorithm. There is no overlap between any inclusions. The center position and Euler angles obey some distribution, as shown in Figure 7.

Figure 7:
Particle/matrix model under shock wave

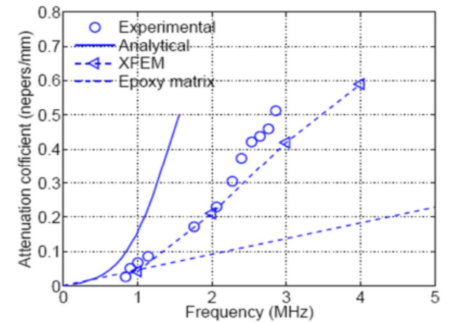


The parameters of glass spheres are $R=150\mu m$, $E=64.89GPa$, $\nu=0.249$, $\rho_g=2.47g/cm^3$. The volume fractions are $V_f=8.6\%$ and 45.1% , respectively. The pressure is $p_0=10MPa$ with $p=p_0\sin(2\pi f t)$. The parameters of viscoelastic matrix are listed in Table 1.

The attenuation coefficient α is computed by the equation given below, which indicates the pressure attenuation from input to output.



8(a)

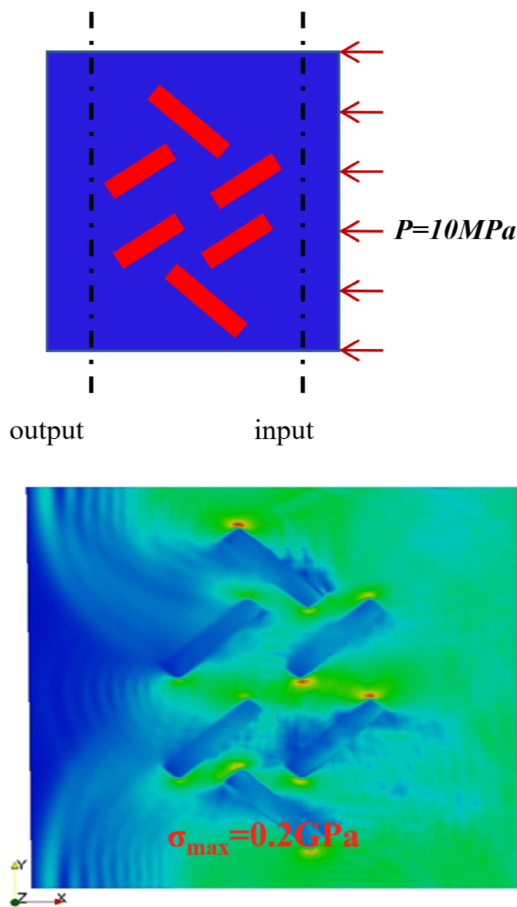


8(b)

Figure 8(a) & (b):
Compared attenuation coefficient with published results

$\alpha = \ln(S_1 / S_2) / (x_1 - x_2)$ nepers/mm, where S_i is a surface of input or output facing the pressure and $x_1 - x_2$ is a distance between the surfaces. For a lower volume fraction 8.6%, as shown in Figure 8(a), there is a little effect on attenuation. While for a higher volume fraction 45.1%, there is significant effect on attenuation corresponding to wave frequencies. The simulation results by XFEM are consistent with the experiment data in Figure 8(b).

Figure 9:
Stress distribution in
fiber/matrix interfacial

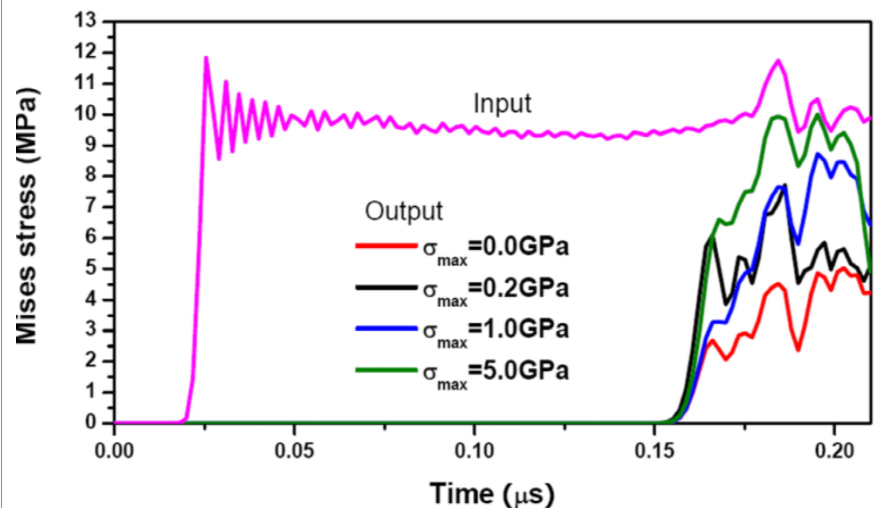


The second example is a 2×2 mm plate (plane strain) given to evaluate the shock wave attenuation mechanism at fibers/matrix interface during shock wave

propagation. There are six short fibers embed in matrix, as shown in *Figure 9*. The stress distribution is plotted by interfacial strength of $\sigma=0.2\text{GPa}$. The parameters of elastic fiber are $E=80\text{GPa}$, $\nu=0.37$, $\rho=2.47\text{g/cm}^3$, $D=100\mu\text{m}$, $L=10D$. The parameters of viscoelastic matrix are listed in *Table 1*.

The shock wave attenuation by interfacial strength is plotted in *Figure 10* as shock period $t=0.8\mu\text{s}$. When interfacial stress is very small, such as $\sigma=0.0\text{GPa}$ (red curve), there are almost 60% pressures attenuated from input (pink curve) [7] corresponding to shock wave could not pass through the interface. ●

Figure 10:
Shock wave attenuation
by fiber/matrix interfacial
strength



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Bridging Scales and Mathematical Models with a Generalized Finite Element Method

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The Generalized or eXtended FEM [1–7] has been developed and improved for more than two decades and is available in several mainstream commercial software such as Abaqus, LS-DYNA, OptiStruct, ANSYS, etc. The GFEM and XFEM are essentially identical methods: the name generalized FEM was adopted by Duarte, Babuska, and Oden in 1995–1998 and the name extended FEM was coined by Belytschko and colleagues in 1999–2000 [8]. The acronym GFEM is adopted in this article. The method removes many of the meshing requirements of the standard FEM, such as fitting meshes to crack surfaces or material interfaces. The generation of these meshes is not trivial and often requires user intervention when dealing with 3-D crack propagation or the evolution of material interfaces. Furthermore, for some classes of problems, such as those governed by the Helmholtz or Poisson equation, the GFEM can deliver accurate solutions using meshes that are much coarser than those required by the FEM [9].

The GFEM is an instance of the Partition of Unity Method [10–13] which is based on two key ideas: (i) The use of a-priori knowledge about the solution of a class of problems to define local approximation spaces; and (ii) The use of a Partition of Unity (PoU) to “paste together” these local approximations. Several families of functions can be used as the PoU: Lagrangian finite element shape functions, meshfree functions such as Shepard and Moving Least Square, B-splines, etc. In the case of the GFEM, the PoU is provided by Finite Element shape functions φ_α , $\alpha = 1, \dots, nn$, where nn is

the number of nodes of an FE mesh. A GFEM shape function is given by the product of a basis functions $E_{\alpha i}$ of a local approximation space and an FE shape function:

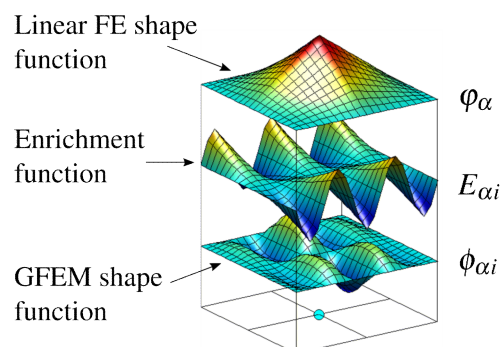
$\phi_{\alpha i}(\mathbf{x}) = \varphi_\alpha(\mathbf{x})E_{\alpha i}(\mathbf{x})$. Figure 1 illustrates the computation of $\phi_{\alpha i}$. The basis functions are often called enrichments. The GFEM has been popular in solving fracture problems. Figure 2 shows a GFEM discretization of a branching crack. The discontinuity across the crack surface is approximated by enrichment functions instead of a mesh fitting it.

What if A-Priori Analytical Knowledge is Limited or Not Available?

Analytical a-priori information is available for many classes of problems, such as Linear Elastic Fracture Mechanics, cohesive fractures (outside of the fracture process zone), material interfaces, acoustic wave propagation, etc. However, in most cases, the available analytical information is limited to simple geometries and physics, for example, 2-D planar cracks with straight fronts. While this limited information can still be used when solving problems with more realistic fracture geometries, mesh refinement is required to compensate for the suboptimal enrichments, as illustrated in Figure 2. For some classes of problems, however, a-priori information may not exist at all. Most nonlinear and multiscale problems fall into this category. The required mesh refinement in this case will be on par with a standard FEM, negating some of the attractive features of the method.

This shortcoming of the GFEM, and in fact of any PoU method, can be removed by adopting *numerically computed enrichments*, instead of relying only on analytical information. Most engineering analyses involve many time or load steps. The idea is then to *use the numerical solution at a simulation step to define enrichment functions for the next step*. Thus, the enrichment functions are produced numerically, on-the-fly, instead of being analytically defined. This allows the use of coarse meshes while still delivering accurate approximations and to bring the benefits of the GFEM to problems that were beyond the scope of the original method.

Figure 1: Computation of a GFEM shape function. Function φ_α is the FE shape function defined on node α of a FEM mesh. It provides the PoU for the GFEM. Function $E_{\alpha i}$ is an enrichment function assigned to node α



Bridging Scales and Mathematical Models with Global-Local Enrichment Functions

Numerically defined enrichment functions are provided by the solution of auxiliary boundary or initial boundary value problems. A global-local analysis is then performed, based on the auxiliary local BVPs and the original global BVP. The GFEM with this class of enrichments is denoted as *GFEM with global-local enrichments* (GFEM^{gl}) [14, 15]. Figure 3 illustrates the application of the method to the simulation of a propagating crack. The solution of the global problem at a propagation step is used to update the crack surface and also to provide boundary conditions for a local problem defined in the neighborhood of the updated crack front. The local problem is solved using the best available numerical method for the quantities of interest. The solution of the local problem, u_L , is then used to enrich the global mesh using GFEM shape functions defined by $\phi_{\alpha}(x) = \varphi_{\alpha}(x)u_L(x)$, where φ_{α} is an FEM shape function from the global mesh. Away from the crack front, analytical information is often available and thus can be used to define GFEM shape functions, as shown in Figure 3. The arrows in the figure show the two-way information transfer between the global and local problems through boundary conditions and enrichment functions – *the method accounts for the coupling between the global and local scales*. This is in contrast with a Global-Local FEM (GL-FEM) analysis, which is broadly used to solve problems with multiple scales of interest [16]. In the GL-FEM, the analysis ends at the local problem – there is no feedback from the local to the global scale. This often leads to large approximation errors, while the GFEM^{gl} can deliver accurate solutions using coarse global meshes like the one shown in Figure 3.

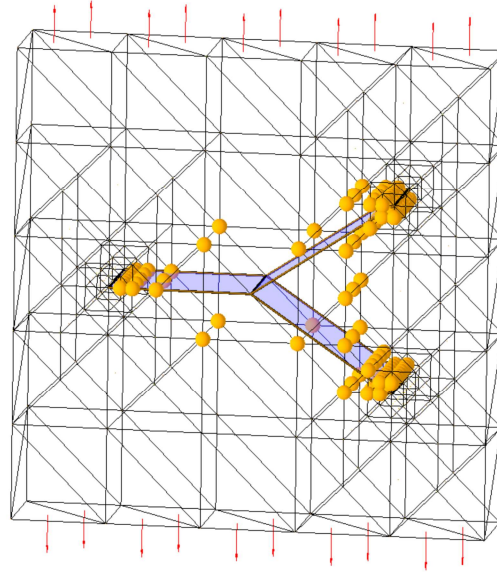


Figure 2: GFEM discretization of a 3-D branched crack. Mesh refinement near crack fronts is required for discretization error control

The GFEM^{gl} offers significant flexibility in the selection of discretization methods for the global and local problems, and also in the choice of mathematical models adopted at each scale. This is important because the most appropriate model for phenomena at the lower scales of a problem is often too expensive and, in fact, not needed everywhere in the analysis domain. As an example, the simulation of crack branching at the scale of local problems can be modeled using peridynamics [17] or a phase field model [18], since these fracture models can robustly model branching. The peridynamics or phase field local solution is then used as an enrichment for the global problem, which can adopt a more computationally efficient model, such as the classical elasticity equations. Another example is the use of enrichment functions provided by a *computational vademecum*, which is pre-computed off-line based on Proper Generalized Decompositions [19].

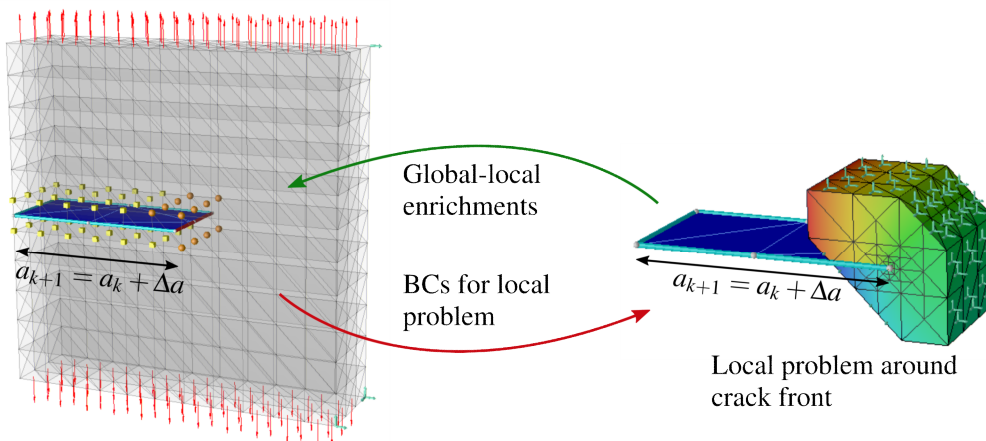


Figure 3: Solution of a crack propagation problem using the GFEM with global-local enrichments (GFEM^{gl}). These functions are computed on-the-fly as the crack propagates. Brown spheres (yellow cubes) indicate nodes enriched with global-local (Heaviside) enrichments

The GFEM^{gl} solution cycle shown in *Figure 3* can be repeated within a time or load step before further advancing the crack. These global-local iterations are used to address the effect of inexact boundary conditions applied to the local problem [20]. Another strategy to address the error in boundary conditions is to solve the local problem in a larger domain with a *buffer zone* while still using the local solution in the domain shown in *Figure 3*. An a-priori error estimate accounting for the effect of inexact boundary conditions applied to the local problem and the size of the buffer zone is provided in [20].

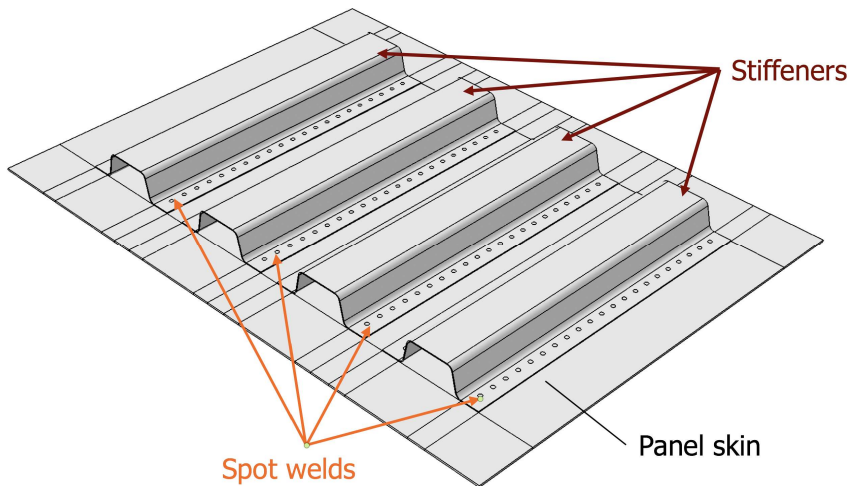


Figure 4:
Hat-stiffened panel with spot welds

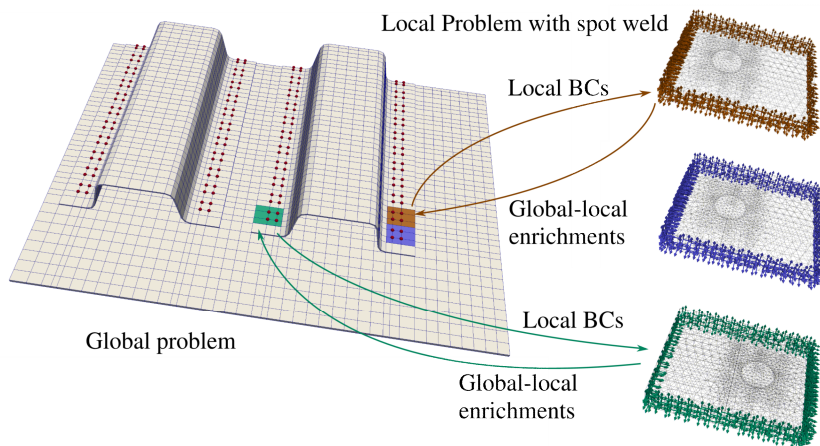


Figure 5:
GFEM^{gl} applied to a hat-stiffened panel. The enrichment functions are provided by the solution of local problems with spot welds. Red nodes of the global mesh are enriched with these functions. They add only three dofs to each node enriched, regardless of the local problem size

Industrial Application: Hat-Stiffened Panel

An example of the application of the GFEM^{gl} to a representative hypersonic structural component is presented next. The CAD model of a hat-stiffened panel is shown in *Figure 4*. The four stiffeners are connected

to the panel skin by 168 spot welds. A fully 3-D model of the welds is often needed to predict damage nucleation and evolution at or near these connections. However, a standard FEM model of a panel and welds usually requires several million degrees of freedom (dofs) [21]. Long duration nonlinear transient simulations based on such models are therefore extremely expensive. Furthermore, the generation of the FEM model is time-consuming. In the GFEM^{gl}, the spot welds are represented using global-local enrichments provided by the solution of local problems like those shown in *Figure 5*. The figure also shows the fairly coarse mesh adopted at the global scale. Only a quarter of the panel is discretized due to symmetries of geometry, boundary conditions and material properties. The welds are ignored at this scale. Thus, the global model is independent of the number and location of the spot welds, which is quite attractive when performing design optimizations. It is also noted that different element types are used at global and local problems, which is convenient when dealing with complex geometries.

A total of 44 local problems are solved in parallel – one for each spot weld. These computations scale very well since there is no communication among local problems during their solution [21, 22]. Their solutions are then used to enrich nodes of the global model, as illustrated in *Figure 5*. This GFEM^{gl} discretization has about 210,000 dofs. The von Mises stress computed at the global problem enriched with these functions is shown in *Figure 6(a)*. Localized stress gradients are well-captured on the coarse-scale mesh and are in good agreement with the Direct Finite Element Analysis results, shown in *Figure 6(b)*. Further verification of the GFEM^{gl} for this class of problems, including time-dependent, nonlinear, and multi-physics responses can be found in [21, 23–25].

Transition to National Laboratories and Industries

A GFEM^{gl} solver can be combined with legacy FEM software using non-intrusive algorithms which require no modifications to the FEM code [26]. This is possible because the GFEM^{gl} can adopt coarse meshes of classical finite elements at the global scale and the local meshes need not be conforming with the global ones as shown earlier. Non-intrusive algorithms provide a pragmatic and fast path for the transition of the GFEM^{gl} to national laboratories and industries. ●

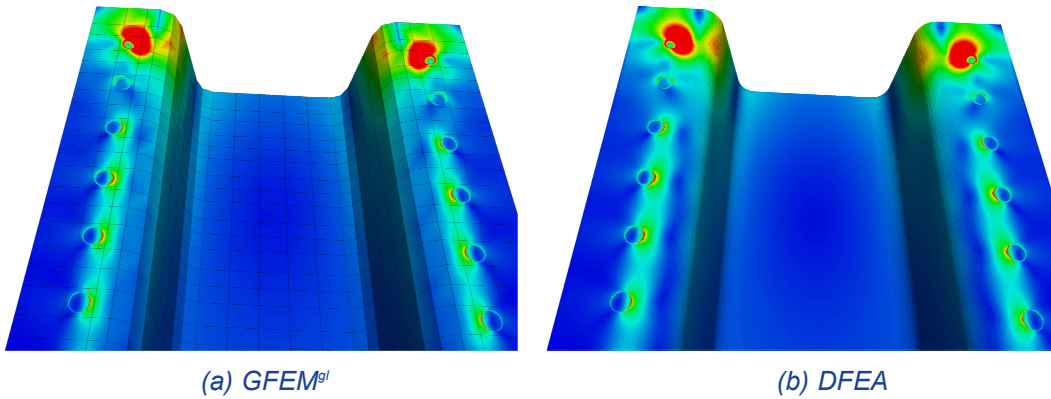


Figure 6: Contour plots of the von Mises stress on stiffeners of the hat-stiffened panel computed with the GFEM^{gl} and from a Direct Finite Element Analysis (DFEA). The DFEA model is about 47 times larger than the GFEM^{gl} model

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Multiscale Modeling of Plasticity in Amorphous & Polymeric Materials

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Amorphous materials are noncrystalline solids that include metallic glasses, glassy polymers, amorphous ceramics, amorphous thin films, some granular materials, and many biological materials, etc, which have widely spread applications in many technology fields. Many of amorphous materials are quasi-brittle and even ductile materials [1, 2] that have high elastic strength with some to significant ductility, and the current trend is to understand the origin of such ductility as well as failure mechanism in order to control material responses and enhance their performance. For instance, metallic glasses can change their ductility/brittleness dependent on the compositions, temperature and thermal history [3, 4]. For amorphous polymers, their glassy state appears below the glass transition temperature T_g , and their rubbery state is above this temperature [5, 6]. Below T_g , the short-range molecular interactions between nonlinked atoms are strong, and local loads are carried from atom to atom. If a small elastic strain is applied to the polymer, almost all carbon-carbon bonds are stretched, and carbon-carbon cone angles are distorted. In the case of large deformation, the atoms (or larger molecular groups) may flip from one position to another, leading to nonrecoverable deformations, or plastic deformation. However, how to quantify such plastic deformation and its consequences is a major challenge in computational materials, because of their complex random microstructure.

Plasticity in amorphous materials is often studied by using molecular dynamics (MD) simulations, [7,8,9,10]. On the one hand, the most accepted phenomenological theory that describes plasticity in amorphous

materials is the Shear-transformation-zone theory (STZ) [8,9,11,12]. However, the STZ theory is an ad-hoc phenomenological defect-mediated flow theory, and it is not a microstructure-specific theory, e.g. it does not take into account the actual disordered microstructure in different amorphous materials, which may result in different inelastic behaviors. Unlike the dislocation-mediate plasticity theory in crystalline solids, presently we know little about the actual amorphous material response process during inelastic deformation, much less about their relations to plasticity and ductile-to-brittle transition. Moreover, the STZ theory may not be suitable to long-chain amorphous polymeric materials. In this article, we discuss our recent work that uses a multiscale method to successfully simulate plasticity in amorphous solids at macroscale [13,14,16].

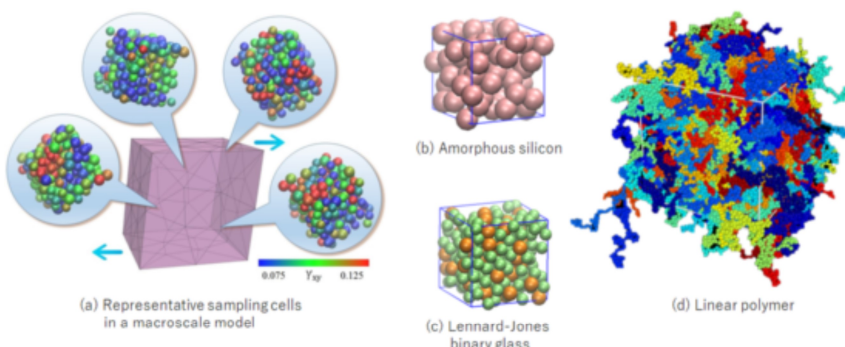
How to define amorphous microstructure

— Representative sampling cell

Our goal is to develop a macroscale plasticity theory in amorphous solids based on microscale rearrangements of atom clusters, defect evolution, and molecular structure change. Contrary to crystalline materials, amorphous materials do not have any definitive microstructure; however, we assume that some typical atom or molecule aggregates may be treated as the representative atomic microstructure for amorphous solids. To accomplish this goal, we couple continuum simulation and amorphous microstructures through representative sampling cells (RS-cells), which contain multiple atoms [13,14,16]. The main purpose of the RS-cell is to intrinsically embed a potential shear-transformation-zone into macroscale material points. For instance, we have built RS-cells for the Lennard-Jones binary glass (LJBG), amorphous silicon (a-Si) and an amorphous polymer material models [13,14,16]. In Figure 1 (a), we show a representative sampling cell for LJ-binary system, in which there are several atom clusters that are marked with different colors, i.e. blue, green, orange, yellow, red, and silver. Figure 1(b) to (d) illustrate the RS-cell for a-Si, LJBG and amorphous polymer model, respectively.

Figure 1:

(a) Representative sampling cell (RS-cell) with different molecular clusters (blue, green, yellow, orange, red, and silver) in a cubic specimen of Lennard-Jones binary glass (LJBG). RS-cells for (b) amorphous silicon, (c) LJBG [13] and (d) coarse-grained linear polymer model [16] (With kind permission of The European Physical Journal (EPJ))



To representatively describe the material response, the number of atoms in a RS-cell is crucial, which is dependent on the material under studied. For LJBG and a-Si, 64 and 250 atoms are minimum [13], while polymer and ionic glasses may require more atoms in order to take into account the chain length and the long-range electrostatic interaction. Before defining such RS-cell, we have conducted a series of large scale molecular dynamics simulations, and determined the minimum size of the RS-cell that can reproduce mechanical responses of a larger atomic model with over 30,000 atoms. A systematic study has been conducted to validate the RS-cell multiscale approach with the full-atom molecular dynamics approach for mechanical responses under various applied loading conditions [13,14].

To reflect statistical variation, a variety of RS-cells should be prepared. To do so, in the case of LJBG model with approximately ten thousands elements, we first construct an RS-cell database that contains 300 RS-cells, and each of them has 250 atoms in a distinct statistically representative configuration [14]. When one starts macroscale finite element calculation, one can randomly select one of the RS-cells from the database as the amorphous microstructure for the quadrature point that is under the consideration.

How to establish an atomistic-informed constitutive relation?

There have been many multiscale models developed for crystalline materials e.g. [17, 18]. A main technical ingredient of these multiscale methods is employment of the so-called Cauchy-Born rule (CBR), which provides a basic rout from microscale to macroscale. In the multiscale finite element methods for crystalline materials, the CBR is applied to a unit cell of a crystal, which is usually “inserted” into quadrature points within an element, and we can utilize this procedure to obtain macroscale stress at those quadrature points, e.g. [19]. However, amorphous materials have no definitive microstructure, one cannot apply the Cauchy-Born rule to a definite microstructure, and this is where the current multiscale method breaks down in the case of amorphous solids.

The key step in our approach is that we employ the RS-cell as the unit cell in amorphous solids to extrapolate stress-strain relation. However, without definite microstructure, there does not exist a fixed

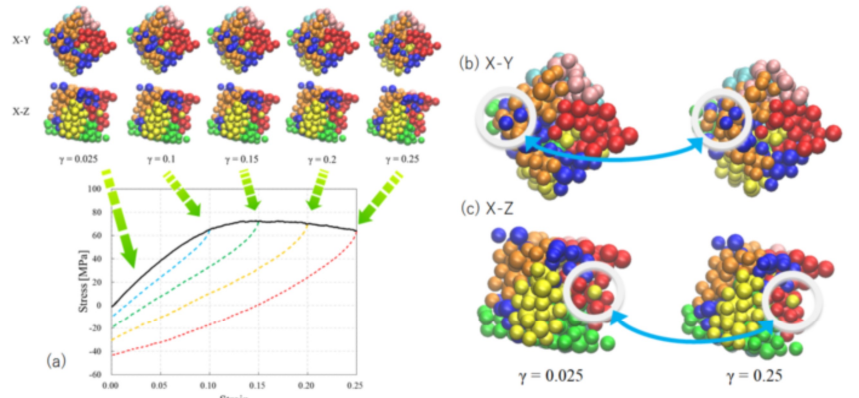


Figure 2: The multiscale connection between microscale shear-transformation-zone evolution in an RS-cell and the macroscale stress-strain relations under pure shear loading. (a) Change of relative positions, local topological arrangements, and configuration of different molecular clusters in an RS-cell corresponding to different strain levels: (b) the local region is centered in a same “blue atom”, and (c) the local region is centered in a same “yellow atom” in a real simulation [14]

atom to anchor the RS-cell, so that we cannot directly apply CBR to derive the macroscale constitutive relation. To overcome this difficulty, we developed the following coarse-grained Parrinello-Rahman (CG-PR) method, which originates from the well-known Parrinello-Rahman molecular dynamics [20,21].

First, we may define an RS-cell shape tensor as

$$\mathbf{h}(0) = [\mathbf{a}, \mathbf{b}, \mathbf{c}], \quad (1)$$

where $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are three edge vectors of the unit cell at initial time, as suggested by Parrinello and Rahman [20]. Following [20], we may use the cell shape tensor $\mathbf{h}$ to re-scales the initial positions of atoms, i.e.

$$\mathbf{R}_i = \mathbf{h}(0)\mathbf{S}_i, \quad i = 1, 2, \dots, N_c, \quad (2)$$

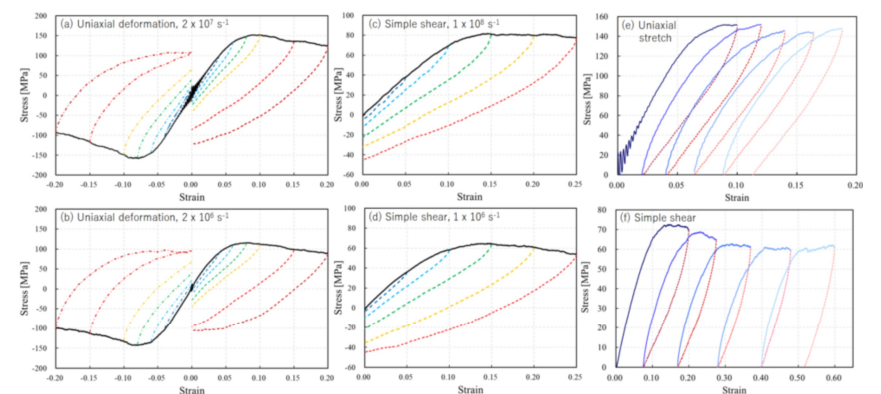
where $\mathbf{S}_i$ is the scaled atom positions.

In macroscale finite element solution, one can find the deformation gradient $\mathbf{F}$ for each element, after nodal displacements are determined for each element. Thus, we can use the CBR to update current configuration $\mathbf{r}_i$ as

$$\mathbf{r}_i = \mathbf{F}\mathbf{R}_i = \mathbf{F} \cdot \mathbf{h}(0) \cdot \mathbf{S}_i = \mathbf{h}(t)\mathbf{S}_i, \quad (3)$$

where $\mathbf{h}(t) = \mathbf{F} \cdot \mathbf{h}(0)$.

Figure 3: Stress-strain loop under cyclic uniaxial loading at with different strain rates obtained by using CG-PR method: (a) $\dot{\epsilon} = \pm 2.0 \times 10^7 \text{ s}^{-1}$, and (b) $\dot{\epsilon} = \pm 2.0 \times 10^6 \text{ s}^{-1}$ (The dotted lines are unloading paths); The stress-strain loop under cyclic shear deformations at different strain rates: (c) $\dot{\gamma} = 1.0 \times 10^8 \text{ s}^{-1}$, (d) $\dot{\gamma} = 1.0 \times 10^6 \text{ s}^{-1}$, and the cyclic loading/unloading hysteresis loops in both uniaxial stretch and shear of the LJ binary glass. (e) Uniaxial stretch: loading rate $2 \times 10^7 \text{ s}^{-1}$, and (f) Simple shear: loading rate $1 \times 10^7 \text{ s}^{-1}$ [14]



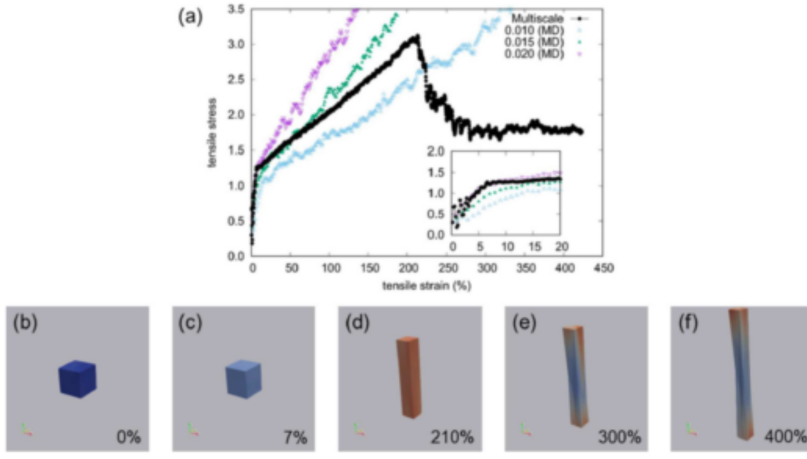


Figure 4:

The tensile stress versus the tensile strain of uniaxially stretched polymeric material obtained from the multiscale simulation (a). The unit of the stress here is $[e/\sigma^3]$, e and σ are the unit of energy and the unit of size of LJ particle in a coarse-grained polymer, respectively. Molecular dynamics simulation results under different uniaxial engineering strain rates (0.01, 0.015, 0.020 $1/\tau$) are also shown in (a). (b) to (f) represent the appearances of the material during deformation at characteristic in (a). Inset in Figure (a) focuses on the transition from elastic to plastic deformation. The color shown in (b) to (f) represents the magnitude of the stress at the local finite element; blue is low and red is high. ([16] With kind permission of The European Physical Journal (EPJ))

For the CG-PR method, we do not solve each S_i explicitly. On the other hand, we use multiscale finite element method to solve $F(t_n)$ for each element at time $t_n = n\Delta t$. In CG-PR computations, the atom configuration ($\mathbf{r}_{gi}(t_n)$) in the current time step n is guessed from previous configuration by using the CBR,

$$\mathbf{r}_{gi}(t_n) = \mathbf{F}(t_n) \cdot \mathbf{R}_i(t_{n-1}) = \mathbf{F}(t_n) \cdot \mathbf{h}(0) \cdot \mathbf{S}_i(t_{n-1}), \quad (4)$$

where, $\mathbf{h}(0)$ is the initial RS-cell shape tensor, $\mathbf{R}_i(t_{n-1})$ is atom coordinate in referential configuration at time step $n - 1$, and $\mathbf{S}_i(t_{n-1})$ is normalized coordinates of atoms in the RS-cell. Once we have initial guess $\mathbf{r}_{gi}(t_n)$, the configuration is optimized to minimize energy by using conjugate gradient method with periodic boundary condition in all directions,

$$\mathbf{r}_i^{opt}(t_n) = \text{argmin}_V(\mathbf{r}_i), \quad (5)$$

with the starting configuration $\mathbf{r}_{gi}(t_n)$.

Finally we can find the correct 1st Piola-Kirchhoff stress as follows,

$$\mathbf{P} = \frac{1}{2\Omega_0} \frac{\partial W}{\partial \mathbf{F}} = \frac{1}{2\Omega_0} \sum_k V'(r_k^{opt}) \frac{\mathbf{r}_k^{opt} \otimes \mathbf{R}_k^{opt}}{r_k^{opt}}, \quad (6)$$

where k is the bond number index.

The ingenuity of the method is to use the shape tensor $\mathbf{h}$ as the motif of the amorphous unit cell, which provides volume change as well as shear deformation measures. Since we embed the RS-cell at the site of quadrature points in a macroscale finite element, when an amorphous material undergoes deformation, each macroscale material point is stressed, and hence each RS-cell is stressed. When the RS-cell is stressed, the atom clusters inside the RS-cell will rearrange their relative positions.

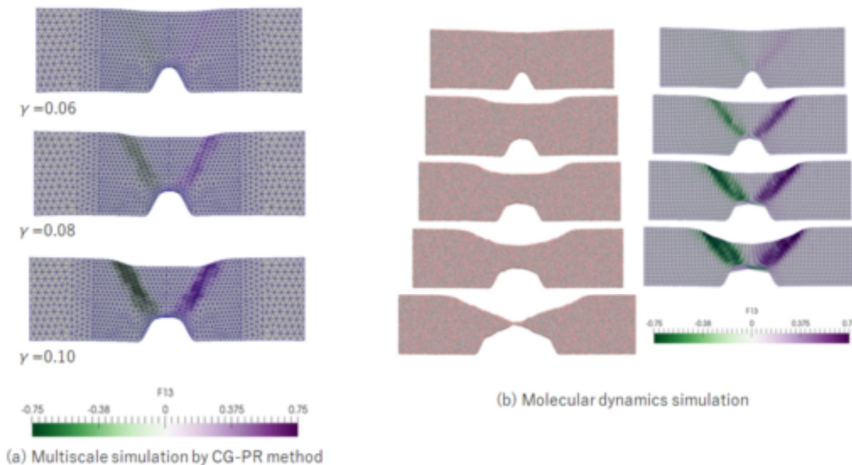
To trace microstructure evolution in an RS-cell, we may divide the atoms in different regions of the RS-cell into distinct regions, and make the atoms in these regions in different colors initially, such as Blue (B), Green (G), Yellow (Y), Organ (O), Red (R), and Silver (S) colors. One can observe from Figure 2, in which a cubic specimen is under shear deformation, the relative positions of atoms, cell volumes, as well as topological connection of these regions (colored atoms) are completely different. Indeed, some of the atoms have larger displacements and thereby create defects following to the macroscale deformation of the specimen. This clearly shows that the multiscale method can automatically acquire shear transformation-zone transition condition, and directly incorporate it into the macroscale flow stress calculation while maintaining the elastic stress level without any empirical inputs.

Multiscale Plasticity

Using the CG-PR method discussed in the above, here we have simulated macroscale plastic deformations in LJBG material as well as an amorphous polymer model. In addition, we have carried out a macroscale simulation that employs millions LJBG RS-cells with continuum finite elements by coupling an open-source MD code, LAMMPS [22], with in-house finite element code.

A challenge in amorphous material research is how to model plastic damage under cyclic loading. Despite of lack of emergence of defect patterns, plastic damage in amorphous can evolve under cyclic loading

Figure 5: Shear band formation in the single-notched specimen of Lennard-Jones binary glass model by using (a) CG-PR method in multiscale manner and (b) molecular dynamics simulations at temperature of 0.2 in Lennard-Jones unit. Right figures in (b) show atomistic view, while left ones in (b) draw strain distributions



and provide a source of kinematically irreversible damage accumulation in amorphous materials, exhibiting fatigue failure under cyclic loading conditions well below the yield stress [23].

Figure 3 shows stress-strain relations under uniaxial loading and shear deformation, and their cyclic deformations were also investigated. If one carefully exams Figure 3 (a)-(d), one may find that the stress-strain (S-S) relations in tension and compression are not completely symmetric, and there are noticeable differences in the yield stresses in different directions. In addition, we find the strain rate dependency of the S-S curves and existence of hysteresis in stress-strain relation. Examining variations of the S-S curves under cyclic loading (see 3(e) and (f)), one may even find the Bauschinger effect. We have also applied the method to simulate plasticity in polymeric materials with long chains. As an example, a multiscale simulation with an RS-cell composed of 100 polymer chains with 100 subsequent beads [15] has conducted, which uses ten thousands of atoms in an RS-cell. Such a large model demands

extensive computations; however, a coupled FEM-LAMMPS code is developed to simulate inelastic deformation of polymers up to one thousand elements, meaning that a multiscale modeling with $100 \times 100 \times 1000 = 10^7$ atoms is now available [16]. Figure 4(a) shows the relation between tensile stress and the tensile strain and (b) to (f) display the appearances of the material at the characteristic tensile strain; 0% (initial state, b), 7% (first yield point, c), 210% (second yield point, d), 300% (lower yield point, e), 400% (final state, f). The tensile stress increases monotonically from (b) to (c) and from (c) to (d). The first yield point (c) is the onset of the plastic deformation and the second yield point relates to the necking phenomena.

The final example is a simulation of shear band formation in a metallic glass. Shear banding is a major inelastic failure mechanism of bulk metallic glasses, and has been studied extensively by experiments e.g. [24], MD simulations and continuum methods [25]. Following [25], we have conducted the CG-PR simulation of the same shape specimen (see Figure 5). The specimen with dimension $3\text{mm} \times 0.1\text{mm} \times 1\text{mm}$ is discretized into 9,344 elements, and each element has an RS-cell composed of 250 atoms of LJBG model. Consequently, the macroscale substrate has freedom of 2,336,000 atoms, resulting a large scale simulation. Figure 5(a) displays shear band formation obtained in a CG-PR simulation, and the result is visually compared with the MD simulation result (352,817 atoms) on the same shape model, whose size is $59.1 \times 9.8 \times 19.7 \text{ nm}^3$ (Figure 5(b)). Further, the simulation result ensures that a coupling of continuum method and computationally efficient parallel code of MD simulator allows us to investigate amorphous materials in a multiscale manner. ●

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Digital & Hybrid Twins: When Data Meets Physics

A new paradigm for simulation-based engineering

by

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I – Simulation-based Engineering

Traditionally, models of materials, processes, structures and systems are expressed from partial differential equations involving numerous parameters. Some of them are related to the physics itself, others describe the geometry of the domain in which the problems are defined, and others are related to the loading and boundary conditions.

Model calibration consists of performing the needed tests and analysis to extract all these parameters. It is at this moment that the problem becomes well posed and its solution is envisaged.

However, the mathematical complexity of the resulting problems makes its exact symbolic solution difficult, and numerical simulation based on discretization becomes the unavoidable major protagonist. Thus, more than looking for the solution at each point in the domain (there is an infinity) at each time instant (another unattainable infinity), we limit our search to a finite number of points (called nodes in the FEM terminology) and some time instants, to later evaluate the solution at any other location and time by simple interpolation. This constitutes an impressive model reduction, much larger than other that have become popular recently and that we will address later.

Discretization leads to linear systems of equations to be solved, sometimes several ones, if we address transient

and/or nonlinear problems. The solution of those linear systems is easily performed by computers. However, the size of these systems (scaling with the number of nodes) and the number of solutions to be obtained (scaling with the number of time steps), makes its fast solution difficult. For this reason, numerical simulation was usually restricted to the design process, where nominal models and loadings (that are expected to represent well the system at hand and the conditions in operation) were solved, leading to nominal designs.

However, at present, with the arrival of new technologies and practices (autonomous cars, connected systems, Internet of Things, ...) simulation is reclaimed in the production workshop, outside the factory, to accompany components and systems all along their life, in operation, in service, ... In some applications the response and feedback characteristic time becomes not compatible with the characteristic time of numerical simulation, making the use of standard techniques difficult.

II – Digital twins

The usual simulation-based route that as discussed consists of using physics-based models, accurately solved by using the just described discretization techniques fails when, during operation, the simulation characteristic time is no more compatible with the process characteristic time.

In this case an alternative route exists. It consists in extracting a model by relating inputs and outputs, both consisting in data. These data could be experimentally measured or synthetic. In the last case, data comes from models solved by using the previously referred expensive numerical simulation. From this data, regression-based metamodels are obtained by making use of advanced machine learning techniques.

*“... certification becomes
compulsory.*

*It seems that, now more than ever,
verification and validation become
critical...”*

Thus, physics-based models will ensure the offline design and sometimes, moreover, the generation of data that will serve to create the data-driven models able to proceed online, under the stringent real-time constraints.

During operation, as soon as data is collected, it can be efficiently assimilated for making predictions and perform preventive and/or operation maintenance.

A new alliance of physics-based and data-driven models can be established and efficiently employed in many industrial applications, with a success that in many cases overpass all the expectations.

III – Beyond digital twins: the hybrid paradigm

The main issues of the just described scenario are:

- In the field of engineering, there is an extraordinary corpus of knowledge, models, ... at the origin of most of the engineering successes of the last century, despite the lack of data;
- In engineering, science and technology, acquiring data is in general expensive (the devices are sometimes extremely expensive). Performing measurements involve in many cases technological difficulties. Finally, in other cases, data is simply unattainable for technical reasons, or because of regulations of different nature. Thus, the use of “smart” data seems more valuable than traditional big-data that applies in other domains, but becomes limited in many areas of engineering, with some exceptions (e.g. data-series, imaging, ...);
- Finally, certification becomes compulsory. It seems that, now more than ever, verification and validation become critical.

We are proving that by hybridizing physics-based and data-driven models, both operating under stringent real-time constraints, the fulfillment of these three requirements becomes possible.

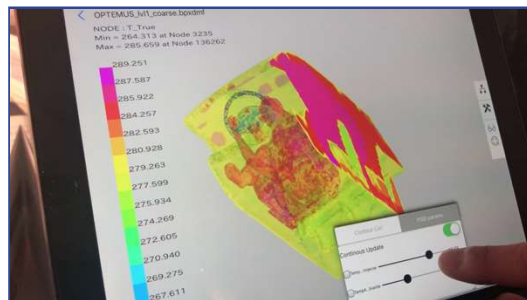
The hybrid paradigm can be expressed as [1]:

Reality = First order physics-based model, manipulated from the tools of applied mathematics and computer science + a data-driven correction, learned on-the-fly, based on data from the use of adequate (engineered) artificial intelligence techniques.

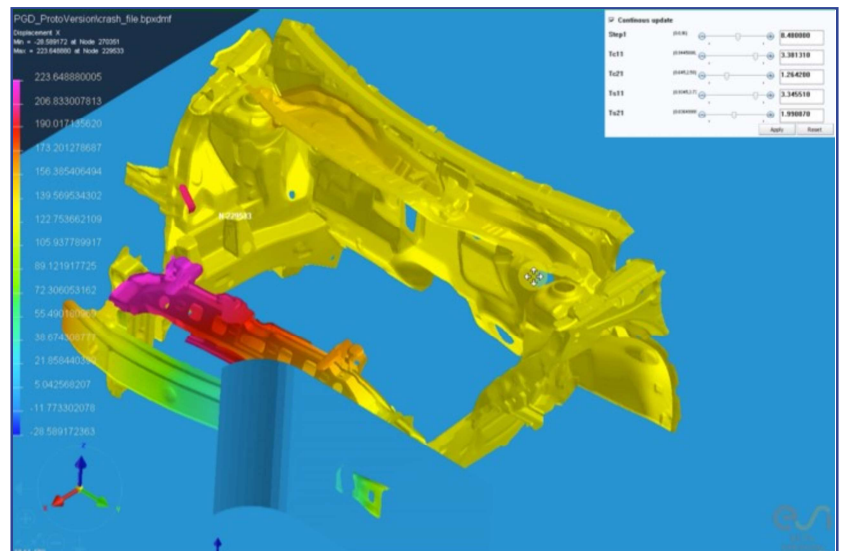
The model enrichment is based on the use of the gap between measurements and model predictions. The interest of using a model is threefold. **First**, it allows moving faster on a sound foundation. **Second**, the better are the models, the smaller are the deviations, implying an almost linear or slightly nonlinear behavior of that deviation, both making possible their approximation from few data. This is in sharp contrast to the vast amount of data needed for creating a model from scratch. Third, if the design is certified from the physics-based model, now the data-driven enrichment acts as a bonus, allowing for better predictions that the ones obtained from the model based on the physics that served for certifying.

Figure 1:

- (a) parametric aerothermal model in car thermal comfort;
(b) parametric crash



(a)



(b)

Advanced Model Order Reduction for efficiently addressing physics-based models

One may think that the solution of physics-based models could be accomplished with the mere use of more powerful computers. Even when this is a valuable route, it makes the accessibility to the appropriate simulation resources challenging. The same happens for its integration in deployed systems. Recent history has proved that this is a critical factor for small and medium-sized companies. Thus, in order to democratize simulation, new solutions are required. Model Order Reduction (MOR) techniques open new possibilities for more efficient simulations [2].

A feasible alternative within the MOR framework consists in extracting “offline” the most significant modes involved in a collection of model snapshots, and then projecting the solution of “pretty similar”

problems in that “reduced space”. Consequently, we must solve a discrete problem of very small size at each iteration or time step. Thus, MOR-based discretization techniques provide significant saving in computing-time—allowing to overcome real-time constraints—. Another MOR-based route consists in calculating offline, using all the needed computational resources (e.g., HPC) and computing time, a parametric solution that contains the solution for all possible (parametric) scenarios.

This parametric solution can then be particularized online to any scenario using mainstream computational facilities, including tablets or even smartphones. With them we will be able to perform efficient simulation, optimization, inverse analysis, uncertainty propagation and simulation-based control—all under real-time constraints—. Such a solution has been demonstrated in many applications where the Proper Generalized Decomposition (PGD) method is used [3].

Figure 2:

*An example of physical-virtual world interaction.
A virtual, rubberlike dragon is manipulated by the user*

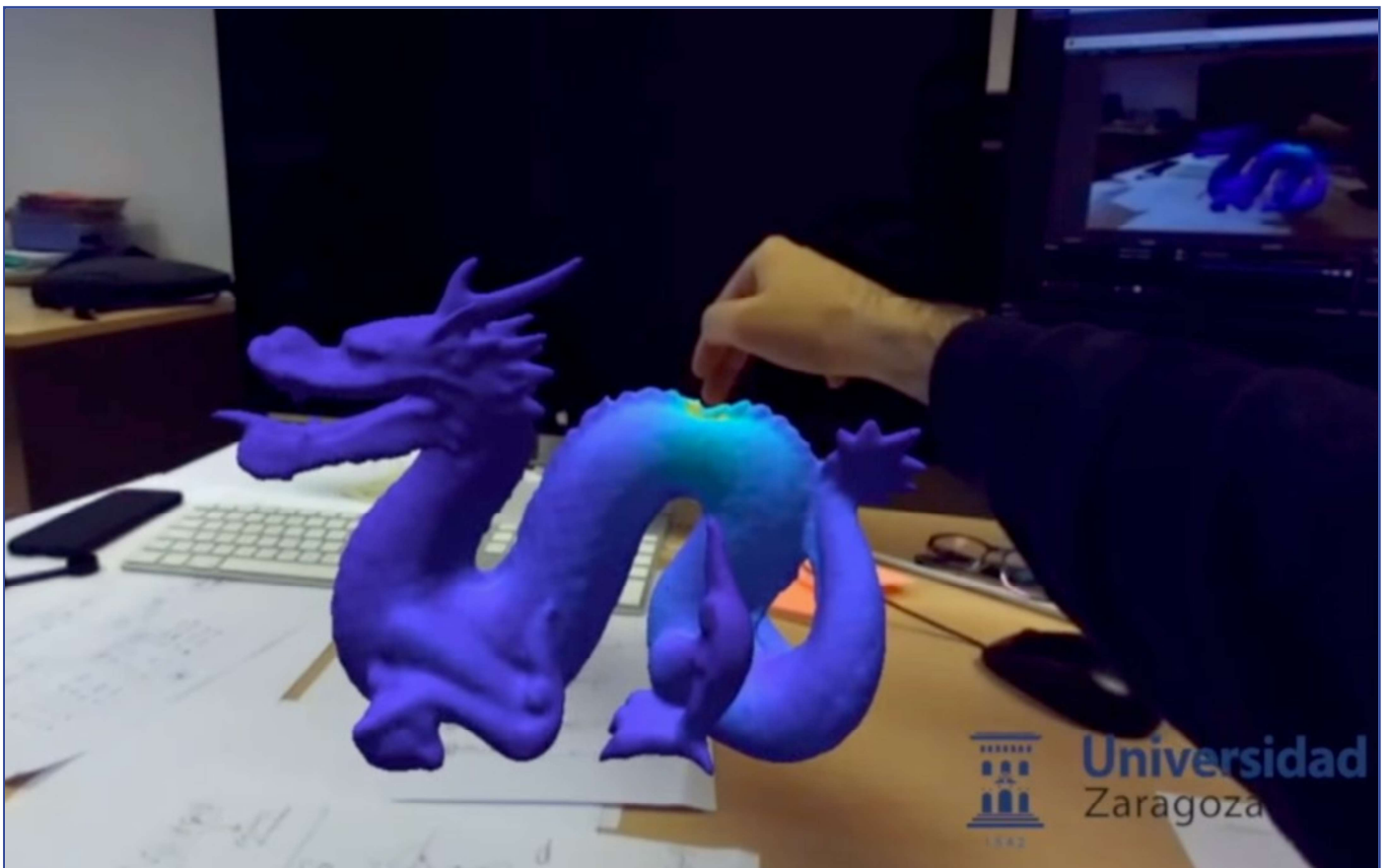
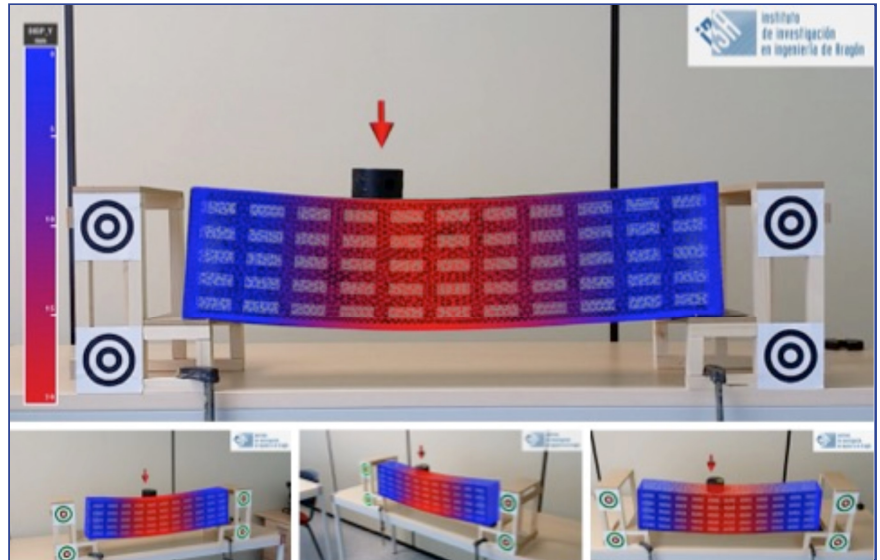


Figure 3:
A hybrid twin for the analysis
and control of a nonlinear
foam beam [12]



The main difficulty of applying the standard PGD constructor just referred is their intrusivity. For circumventing this difficulty and making possible the use of standard solvers for constructing those parametric solutions (also called virtual chars or vademecums) one can apply robust interpolation or regression techniques operating on the snapshots coming from high-fidelity solutions for different values of the model parameters. Special care must be paid for ensuring the scalability of those techniques with the number of parameters and for providing error estimators/indicators.

A first proposal, called SSL–Sparse Subspace Learning—, allowed the construction of parametric solutions when the number of parameters remained moderate [4]. Later, the so-called sparse PGD (s-PGD) allowed increasing the number of parameters, with, in many cases, an almost linear scalability of the number of snapshots with respect to the number of parameters involved in the model. Its main ingredients are the separated representation, the sparsity (inspired of sparse sensing [5]) and the use of kriging to avoid large oscillations when constructing interpolations from arbitrary collocation points [6].

Even if, in many cases, parameters involved in a model are quite natural, in other cases are much less evident. For example, when considering physics depending on parametrized shapes. In that case, advanced nonlinear dimensionality reduction techniques allow to extract the minimum number of explicative uncorrelated parameters, sometime involving complex combination of them. We proved in [7,8] that when addressing the mechanics of organs (e.g. human livers) or car aerodynamics (depending on the cars shape) few parameters suffices, facilitating the construction of parametric solutions.

Figure 1 depicts the use of two parametric solutions, both constructed by using the sPGD.

Engineered Artificial Intelligence

When data is abundant and we proceed offline, the use of deep-learning is an excellent candidate. However, when data is very scarce and the data-driven model must adapt in time very fast, other techniques able to operate in these circumstances could and should be considered, analyzed, developed, improved and tested on real use cases.

This analysis constitutes the main purpose of the so-called Engineered AI that embraces: (i) visualizing multidimensional data; (ii) classifying data; (iii) modeling the input / output relationship enabling quantitative predictions; (iv) certifying those predictions; (v) explaining them—that is, extracting knowledge from the available data—, and (vi) applying them in service (taking advantage of the online adaptation or hybrid paradigm) and training final users or even students on the use of AI techniques for adding value to industrial technology.

Some advanced modelling techniques concern:

- (i) sparse-multi-local-multi-parametric non-linear regressions working at the low-data limit [6];
- (ii) the combination of dynamic mode decomposition (DMD) with reduced modelling leading to the incremental-DMD (iDMD) [9];
- (iii) techniques able to proceed with heterogeneous data (categorical, discrete, qualitative, ...) by mapping them from a representation space to a vector space [10];

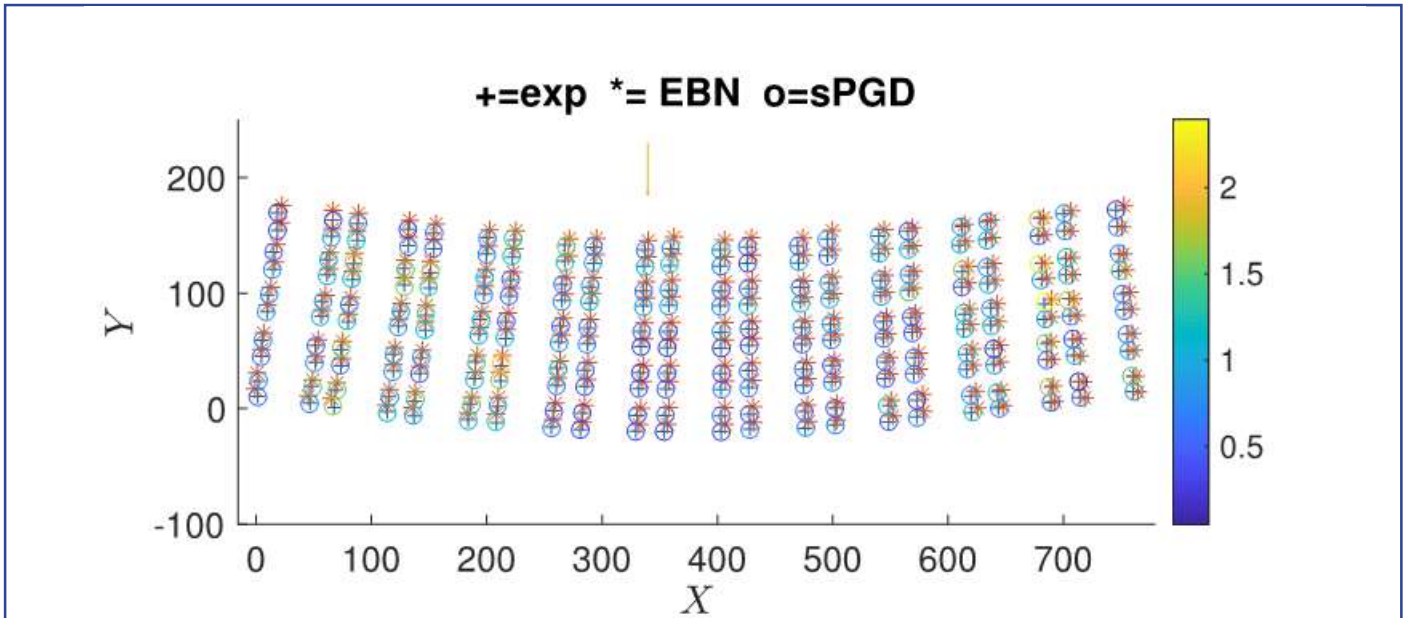


Figure 4:
 Experimental measurements (denoted by “+” symbols),
 Euler-Bernoulli-Navier prediction (asterisks) and self-corrected model by
 s-PGD methods, denoted by open circles.
 The legend represents the absolute error, in mm.
 These values can be lowered by improving the resolution of the camera (placing it closer
 to the beam, for instance).

(iv) the introduction of physics into the learning process, specially appealing when addressing mechanical systems obeying the principles of thermodynamics [11]; and (v) the use of appropriate metrics (other than the Euclidean) for performing machine learning, one promising framework being the Topological Data Analysis [11], crucial for describing and parametrizing complex morphologies and topologies.

Virtual, Augmented and Mixed reality

The just mentioned capabilities of hybrid methodologies pave the way for the development of physics-based virtual, augmented and mixed reality applications. Video streams run at some 30-60 frames per second, so it is now possible to develop simulation apps that, running in the background, obtain predictions for decision making, assimilate data or even interact with the physical “reality”. In Figure 2, for instance, we show an example of virtual-physical worlds interaction. It shows how a (virtual) rubber dragon deforms under a virtual manipulation.

IV – Illustration

To illustrate the capabilities of a hybrid

twin, consider, for instance a foam beam, shown in Figure 3. We constructed a hybrid twin of the beam with the help of (i) computer vision for data acquisition (ii) a classical Euler-Bernoulli-Navier (linear) beam model (iii) augmented reality for assisting in decision making processes.

The twin is able to detect systematic biases among measurements (displacement) and predictions given by the simple model. By employing sparse-PGD, the model can be corrected by the twin itself without any human intervention. This correction, thanks to the s-PGD methodology, involves very scarce data and a minimum number of measurements [12]. In addition, the twin performs data assimilation in real time. In this case, see Figure 3, it is able to locate the position of the load (see the red arrow) and correct the assumed model if it renders systematic errors.

The next natural step is including the human in the loop, but for that knowledge must be approached in a more systematics and rational way, by certainly constructing a multi-scale theory of data, a sort of thermodynamics of data, where entropy will become again a major protagonist [13].

V – Final remark

As Einstein claimed, it is difficult to change the paradigm from within. In other words, imagine the consequences if the now-days computing revolutions in 40 or 50 years. Gauss claimed that we, now, are a sort of clowns for people observing us in the future. Napoleon invited Alessandro Volta to the French Academy of Sciences, to show the actions of the just discovered electricity (provided by his battery) on some frogs that jumped by the action of the applied electrodes. At the end of the exhibition Napoleon asked Volta: – Do you think that the so-called electricity could serve a day to something other than inducing jumps to frogs?

We are totally persuaded that concerning artificial intelligence we are at the stage of Volta's frogs. Something incredible and unimaginable for us will come, but this time it is not necessary to attend one

century. The use of all this power will depend, once more, on us. Technologies are not good or bad: it is their use what matters, and this is our responsibility.

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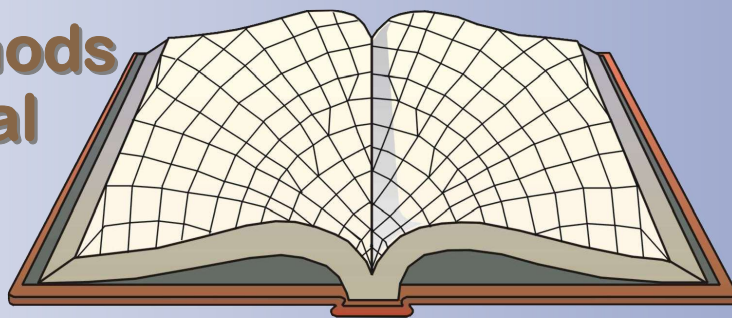
“The use of all this power will depend, once more, on us. Technologies are not good or bad: it is their use what matters, and this is our responsibility.”

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Reduced Basis Methods for Partial Differential Equations

Alfio Quarteroni, Andrea Manzoni
& Federico Negri
Springer, Switzerland, 2016



BOOK

REVIEW

ISBN: : 978-3-319-15431-2, 296 pages, soft cover, £52 (List Price)

Contents: Preface; 1: Introduction; 2: Representative Problems: Analysis and (High-Fidelity) Approximation; 3: RB Methods: Basic Principles, Basic Properties; 4: On the Algebraic and Geometric Structure of RB Methods; 5: The Theoretical Rationale Behind; 6: Construction of RB Spaces by SVD-POD; 7: Construction of RB Spaces by the Greedy Algorithm; 8: RB Methods in Action: Setting up the Problem; 9: RB Methods in Action: Computing the Solution; 10: Extension to Nonaffine Problems; 11: Extension to Nonlinear Problems; 12: Reduction and Control; Appendix A: Basic Theoretical Tools; References; Index.

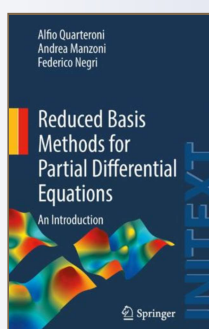
This book was published in the Springer series "UNITEXT – La Matematica per il 3+2", which is designed for undergraduate and graduate academic courses, and also includes advanced textbooks at a research level, like this one. The series was originally released in Italian, which explains its title. The Editor-in-Chief of the series is the well-known computational mathematician Alfio Quarteroni, who is also the senior author of this book. The other two authors are young researchers from his former group in EPFL, Lausanne (now Prof. Quarteroni is based at the Politecnico di Milano).

The subject of the book is Reduced Basis (RB) methods for parametrized PDEs. These methods constitute a branch within the larger area of Reduced Order Modeling (ROM). The latter has become a major area of interest in recent years, which many research papers and conference sessions are dedicated to. The general idea of ROM is to replace a “heavy” numerical model, called here a “high fidelity” model, with a much more efficient model which retains the same level of accuracy in some desired sense. This general setup has several variants, one of which is the subject of this book.

The particular scenario under investigation here is that of a problem governed by a PDE which involves a set of parameters. One is interested in solving the problem repeatedly for many different values of these parameters. For a very large number of degrees of freedom, say $O(10^6-10^9)$, the computational cost of solving all these many problems, using a standard numerical method with appropriate resolution, is prohibitive. The book discusses RB methods, in a variational setting, for solving these problems efficiently, while still obtaining accurate solutions. The idea underlying Galerkin and Petrov-Galerkin RB methods, on which the book concentrates, is the projection of the high-fidelity problem on a subspace spanned by specially chosen basis functions. The subspace is constructed via a relatively small number of representative high-fidelity solutions, called “snapshots”, for a small number of parameters. The dimension of the resulting reduced system of equations is related to the number of snapshots.

The book provides the basic mathematical understanding and tools for RB methods. It does that very successfully: it is mathematically rigorous but not dry at all, fully covers the theory but also provides practical algorithms with full details, as well as helpful discussions. The notation is simple and clear. Still, a list of symbols at the beginning of the book would have been helpful

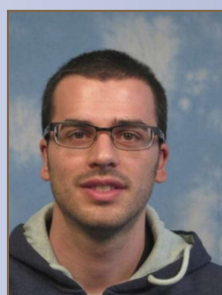
(perhaps in the 2nd edition). The book is not only well written, but is also excellently edited, and very pleasant to the eye: definitions, theorems, etc. are written on a darker background, algorithms are written in boxes, and there are a decent number of figures, some of them in color. Each chapter ends with several well-designed exercises.



Alfio Quarteroni



Andrea Manzoni



Federico Negri

The list of references at the end of the book is comprehensive.

It seems to me that a reader without good background in functional analysis (despite Appendix A, which serves as a reference to the basic concepts) and variational formulations will find the book hard to read. On the other hand, readers with sufficient background in these areas, like many mathematically-oriented members of the Computational Mechanics community, will enjoy the book and benefit a lot from it.

The Introduction provides a number of examples for parametrized PDEs, including interesting problems in optimal control, shape optimization and certain types of inverse problems.

After presenting the problems at the continuous level, the authors describe them at the discrete level, and explain the need for reduction. Then the basic theory of RB methods is briefly outlined. An important distinction is made here between offline and online computations.

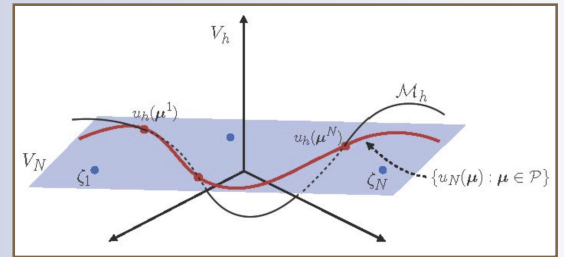
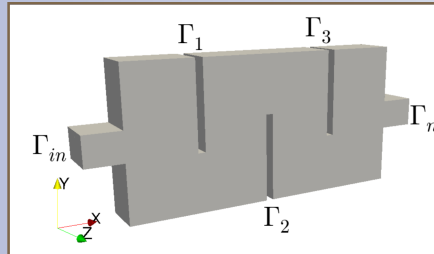


Figure 1:
The snapshots, the manifold and the RB space. This is Fig. 3.1 in the book

The concept of affine parametric dependence is also defined here. This is a situation where the stiffness matrix and load vector depend on the parameters in a "scalar" way. In this case one achieves high efficiency in the assembly of the arrays at the online stage. Most of the book chapters assume the affine dependence property, but Chapter 10 is dedicated to the extension of RB methods to the non-affine case.

Chapter 2 is a fine treatment of a number of representative problems, which are used to demonstrate the RB methodology throughout the book. All of them are elliptic – time-dependent problems are not discussed. These include (1) and advection-diffusion-reaction problem, (2) linear isotropic elasticity, (3) Stokes flow, and (4) steady-state Navier-Stokes (NS) equations for incompressible flow – an example of a nonlinear problem. Section 2.2 provides some tools for variational formulations. An important classification of problems is made, including strongly coercive problems, weakly coercive problems (which are inf-sup stable), and saddle-point problems. The latter category is a special case of the second category, and as we know from the Babuška-Brezzi theory for mixed Finite Element (FE) formulations, it is a hard nut to crack. In Section 2.3 the authors analyze the well-posedness of the three linear problems defined previously in view of that classification. Section 2.4 is the analogous discussion at the discrete (algebraic) level. Chapter 2 ends with a short discussion on FE spaces.

Chapter 3 is the heart of the book: here RB methods are developed in their full glory, for the general case of inf-sup stable operators. One starts with a set of snapshots for a few parameter sets. Then the RB is constructed by orthonormalization of the snapshots with respect to an appropriate inner product. *Figure 1*, which is Fig. 3.1 from the book, illustrates the process abstractly. In addition to the Galerkin RB method, the Least Squares RB method is presented (which can be viewed as a special case of a Petrov-Galerkin RB method). Here too the methods are discussed first at the continuous level and then at the discrete level. The efficient implementation of the online process in the case where the discrete operator is affine is explained, and *a posteriori* error estimates are given. The chapter ends with a solved problem of advection-diffusion. *Figures 2 and 3* appear in the book in this context.

This chapter includes a few algorithms which are nicely presented. In most of them the authors indicate, at the side of the algorithm boxes, the complexity (number of operations) associated with each of the loops involved, e.g., $O(N^2)$. This is a very nice and helpful feature that I have never seen in any other book before.

In Chapter 4 the authors show the algebraic properties of the various RB methods and their geometric interpretation (which "justifies" the use of the terms projection and orthogonality). Chapter 5 is for the "advanced", and is the most mathematical chapter in the book, although the questions asked here are quite practical and important: When is a problem reducible? How good

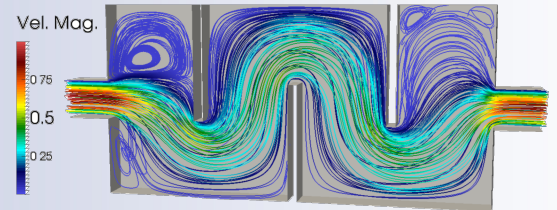


Figure 2:
Geometry and Navier-Stokes streamlines as input of an advection-diffusion problem. This is Fig. 3.2 in the book

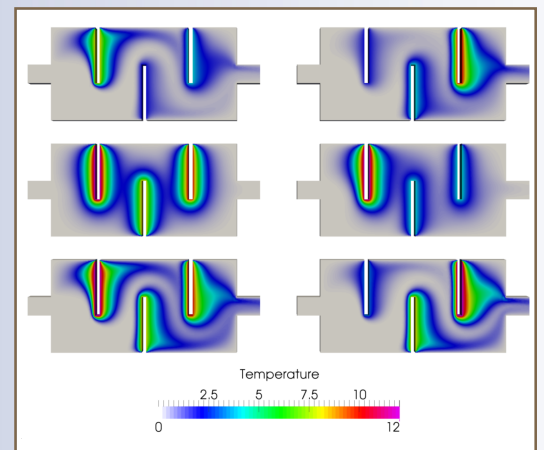


Figure 3:
RB solutions of the problem of Fig. 2, for different sets of parameter values. This is Fig. 3.3 in the book

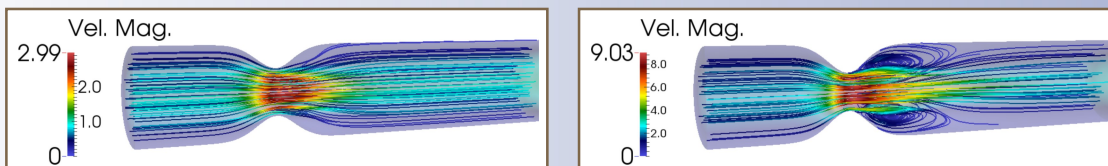
is the approximation of the solution manifold? How small can the dimension of the RB space be? Alas, the answers to these questions require heavy mathematics, which culminates in the use of the Kolmogorov n -width.

Chapter 6 is a very nice treatment of the construction of the RB space via SVD and Proper Orthogonal Decomposition (POD). POD is a popular way to implement the procedure presented in Chapter 3 at the discrete level. As an introduction to this topic, the authors explain how to find, using SVD, the best approximation of a matrix by a matrix of a lower rank (this is the SEY theorem). They discuss the use of SVD for two applications: image compression and data mining using the Principal Component Analysis (PCA) approach.

Chapter 7 focuses on the construction of RB spaces using a greedy algorithm, which is different than POD. An optimization algorithm is called greedy if in each iteration it finds a locally optimal solution. In the context of RB methods, a greedy algorithm is a procedure which constructs the space by adding a single vector to the basis in each step. This amounts to searching, in each step, a snapshot which is the *worst* approximation of the current RB subspace. The chapter includes an error analysis of the method.

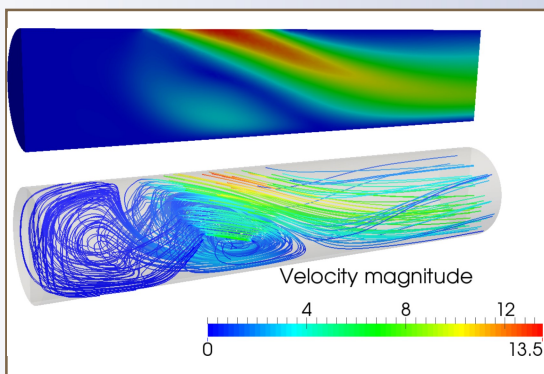
The RB procedure presented in Chapter 3 requires that the computational domain will not involve varying parameter values. Chapter 8 shows how to transform a problem in a general domain to a problem associated with a reference domain that does not involve varying parameters. The procedure is applied to an example of advection-diffusion-reaction. A side comment on this example is that some known parameter values are given as numbers (e.g., 100 appearing in the expression of the thermal conductivity) rather than as symbols. It would have been preferable to avoid using numerical values in the examples, although I am aware that using only symbols may lead to lengthy expressions.

Figure 4:
Representative RB solutions for a problem of a sudden expansion channel. This is part of Fig. 11.4 in the book

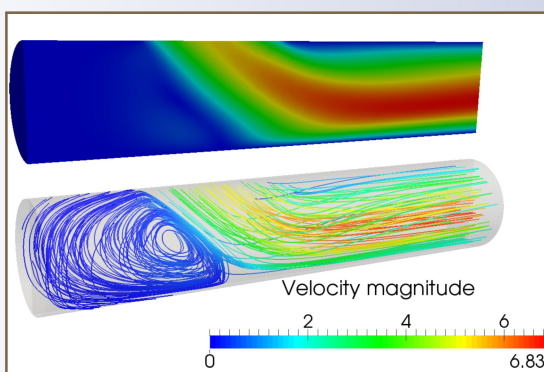


Chapter 9 contains numerical examples for linear affine problems. Chapter 10 discusses the extension to non-affine problems. The main algorithm to this end is the empirical interpolation method (EIM). A variant of EIM, called DEIM, where the development is done from the outset at the discrete level, is also discussed. The comparison between the two is related to the general question of which way to go – apply the computational method at the continuous level and

then discretize, or first discretize and then apply the method. I think that theoretically one should always prefer the former, since it usually provides more mathematical insight. However, sometimes discretizing from the outset is so much simpler to perform that one is tempted to sacrifice the mathematical insight.



Chapter 11 deals with the major extension of RB methods to nonlinear problems, and in particular to the NS equations and to a semi-linear elliptic problem. The RB approximation is combined with the Newton method that linearizes the problem iteratively. Chapter 12 discusses problems of constrained optimization and optimal control, and shows how the RB technique can be used very effectively for such problems. These last two chapters include impressive numerical examples; see *Figures 4 and 5*.



In summary, this is an excellent book, highly recommended to readers with solid mathematical background, on RB methods for an important class of problems, namely those governed by parametrized PDEs. The material covered is very relevant to researchers and graduate students interested in ROM in general, and is presented in a very effective manner. ●

Figure 5:
Solution of an optimal control problem with the initial parameter value (top) and the optimal value (bottom). This is Fig. 12.3 in the book

for all inclusions under
APMTAC please contact:
Jose Cesar de Sa
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CMN2019 (Congress on Numerical Methods in Engineering) took place in July 2019 at Guimarães, Portugal. CMN 2019 was a great forum for the discussion of relevant scientific, and technological developments in computational mechanics, numerical methods and engineering applications.

CMN2019 was jointly organized by the Portuguese (APMTAC) and the Spanish (SEMNI) Associations and followed the mutual congress editions of Madrid (2002), Lisbon (2004), Granada (2005), Porto (2007), Barcelona (2009), Coimbra (2011), Bilbao (2013), Lisbon (2015) and Valencia (2017).

The scientific program comprised of six plenary lectures from internationally known researchers and was structured in almost 30 thematic sessions of different fields of research. The topics covered ranged from discrete modelling to fluid mechanics, including multi body dynamics and finite elements, applied to different fields ranging from civil engineering to biology. More than 275 participants from 30 countries were present at CMN 2019, making it a truly international event.

It should be noted that young participants (MSc and PhD students) totaled about 40% of the attendees, demonstrating that the future of this community is promising. Thinking about the young participants, a unique presentation possibility was offered with oral (more formal and less interactive) and poster (informal and interactive) presentations of the same paper. This edition of the CMN also included one day-training courses on different advanced software packages, which more than 50 participants in total.

Following on the tradition of great social programmes, this edition was no exception, with engaging events in one of the most important historical cities in Portugal, having been declared World Heritage Site by UNESCO in 2001. During the gala dinner, at a location with prime panoramic view over the city, the awards ceremony, given by the APMTAC and SEMNI took place, which included Career and Recognition Awards, as well as Young Researchers and PhD Thesis Awards.

At the end of this year's event, the next organizing team had a chance to present the venue for the CMN2021. Grand Canaria was chosen to host the next conference of this series. ●



Figures 1 & 2:
Overview of the opening ceremony at CMN2019



Figure 3:
APMTAC Board Meeting at CMN2019



Figure 4:
SEMNI Olgierd Zienkiewicz Award to
Prof. Manuel Doblaré

by
Tobias Gleim
Stephan Lange

8th GACM Colloquium on Computational Mechanics 28-30 August 2019 in Kassel



Figure 1:
GACM President Michael Kaliske and the
5 plenary speakers Antonio Huerta,
Peter Betsch, Jörg Schröder,
Bettina Schröder and Steffen Rothe



Figure 3:
Conference Chairmen
Tobias Gleim (left) & Stephan Lange (right)



Figure 4:
The three GACM
Best Ph.D. Award
winners 2017 & 2018
and the GACM
President (f.l.t.r.
Johanna Waimann,
Silvia Budday,
Michael Kaliske,
Dominik Budday)

Figure 5:
Conference banquet
at Kulturbahnhof
of Kassel



The 8th GACM Colloquium on Computational Mechanics for Young Scientists from Academia and Industry was hosted by the Chair for Mechanics and Dynamics of the department for civil and environmental engineering and by the Chair for Technical and Continuum Mechanics of the department for mechanical engineering of the University of Kassel. Around 180 participants from 14 countries including doctoral students, post-docs, professors and students created a lively and friendly atmosphere having many fantastic talks and even more fruitful discussions. 155 presentations were organized in 21 mini-symposia and held in 33 parallel sessions. The contributions of young researchers were supplemented by four plenary lectures by renowned experts from science and industry. Antonio Huerta gave an inspiring lecture on low and high-order approximations for computationally-demanding problems, Peter Betsch talked about important topics in the context of energy-momentum-entropy schemes, Jörg Schröder explained crucial phenomena in the characterization of magneto-electric composites and Bettina Schröder and Steffen Rothe from Volkswagen AG gave insights about current challenging research topics and their implementation. In addition, Silvia Budday, Johanna Waimann and Dominik Budday, the three GACM Best Ph.D. Award winners of the years 2017 and 2018 could present their Ph.D. thesis to the plenary auditorium.

In the poster session, many valuable discussions took place and the four winners of the GACM Best Poster Award were nominated in a thorough evaluation procedure by the GACM board and all plenary speakers. During the welcome reception on the first evening, the GACM Best Poster Awards were announced to the auditorium and handed over to Ivo Steinbrecher, Sonja Uebing, Veronika Straub and Dominik Horny by the GACM President Michael Kaliske. The valuable mini-symposia were complemented by social events to strengthen the exchange in additional discussions in the community by the participants. The banquet took place at the south wing of the Kulturbahnhof of Kassel, a former postal center. The culinary meal was served on a former railway track. Otto Bruhns gave a very entertaining dinner speech about his time in the 80s at the University of Kassel and its very interesting peculiarities.

Overall, the 8th GACM Colloquium on Computational Mechanics in Kassel was a great success and will be succeeded by the 9th Colloquium to be held at the University of Duisburg-Essen in 2021. ●

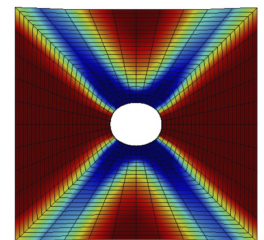
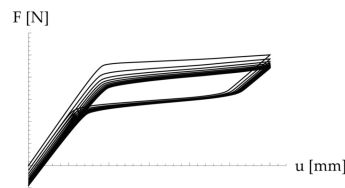
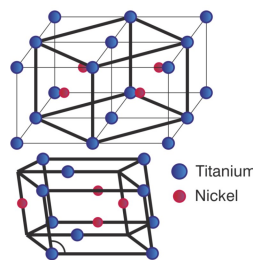


GACM Best PhD Awards

It is a great pleasure to announce that the two outstanding doctoral theses of **Dr.-Ing. Johanna Waimann** and **Dr.-Ing. Dominik Budday** were honored by the GACM Best PhD Award 2018 on the occasion of the 8th GACM Colloquium on Computational Mechanics in Kassel. Dr. Waimann's thesis on "**Variationelle Modellierung irreversibler Effekte in polykristallinen Formgedächtnislegierungen**" was supervised by Prof. Hackl at Ruhr-Universität Bochum. Dr. Budday conducted his work on "**High-Dimensional Robotics at the Nanoscale — Kino-Geometric Modeling of Proteins and Molecular Mechanisms**" at Friedrich-Alexander-Universität Erlangen-Nürnberg under the academic supervision of Prof. Leyendecker.

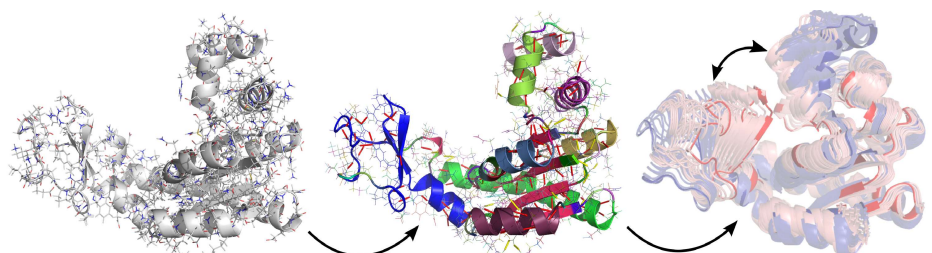
Dr.-Ing. Johanna Waimann: "Variationelle Modellierung irreversibler Effekte in polykristallinen Formgedächtnislegierungen"

In her thesis, Johanna Waimann deals with variational modeling of irreversible effects during the solid/solid phase transformation in polycrystalline shape memory alloys. Based on the principle of the minimum of the dissipation potential, three models are presented to show the so-called effect of functional fatigue. The first two models couple the phase transformation between the austenitic and the different martensitic variants with plasticity or, respectively, with the formation of irreversible martensite. Thereby, the simultaneous evolution of the microstructural effects is considered by a coupled dissipation function. To also examine the influence of thermal cycling, the third material model saves the transformation history of the body. In her thesis, Johanna Waimann also examined different approaches to account for the polycrystalline structure of the material: a combined Voigt/Reuß energy bound resulting in a grain-wise evolution of the microstructure and a dynamically evolving orientation distribution function for a computationally more efficient calculation. Several simulations – on the material point level as well as using the finite element method – and a comparison to experimental data, proof the functionality of the models.



Dr.-Ing. Dominik Budday: "High-Dimensional Robotics at the Nanoscale — Kino-Geometric Modeling of Proteins and Molecular Mechanisms"

Proteins are dynamic biomolecules that perform a tremendous variety of cellular functions on a broad range of spatio-temporal scales, demanding efficient, yet elaborate integrative computational methods to resolve their motions. In his thesis, Dr. Budday lays out a robotics-inspired, kino-geometric modeling and sampling approach to capture small- and large-scale protein collective motions. He develops a universal theory for geometric rigidity analysis, decomposing macromolecules into larger rigid substructures in a matter of seconds. The remaining coordinated motions form the basis for a high-dimensional motion planning algorithm termed dCC-RRT, which integrates the principle of minimal frustration via dynamic, Clash-avoiding Constraints (dCC) into a rapidly-exploring random tree (RRT). The algorithm closely approximates conformational transitions and agrees well with motions from Molecular Dynamics simulations and experimental data. Via large-scale, multi-dataset benchmark analyses, Dr. Budday further demonstrates how the model captures highly conserved, protein fold specific, dynamic information that often enters undetected in comparable methods. The developed tools provide a robust and efficient alternative to obtain high-level insights into molecular mechanisms across scales, with broad applications in protein engineering, drug design, and human health. ●



by
Michael Kaliske
(GACM President)
Ines Wollny
(Secretary General,
GACM)

5th German-Japanese Workshop on Computational Mechanics

On September 23 and 24, 2019, all together 34 Scientists from Japan and Germany met at Technische Universität Dresden for the 5th German-Japanese Workshop on Computational Mechanics. The aim of this successful workshop series is to intensify the scientific relationship between senior and junior German and Japanese researchers in the broad field of computational mechanics. The workshop was organized by Prof. Michael Kaliske, head of the Institute for Structural Analysis and current President of the German Association for Computational Mechanics (GACM), in cooperation with the Japan Society for Computational Engineering and Science (JSCES) and partly financially supported by TU Dresden and GACM. The previous four workshops in this series took place in Sendai, Japan (2017), München, Germany (2015), Yokohama, Japan (2010) and Hannover, Germany (2004).



Figure 1:
Group photo of 5th
German-Japanese
Workshop

The scientific program comprised 19 talks on up to date research topics in the wide field of computational mechanics given by senior and junior scientists from Japan and Germany and fruitful discussions. The program was topped off with a sightseeing walk through the old city center of Dresden, the conference banquet, which was held in a historic vault of the restaurant “Sophienkeller”, as well as a trip by an old-timer bus to the winery “Schloss Wackerbarth”. It was a great pleasure to host this workshop and welcome our friends from Japan in Dresden. We are already looking forward for the 6th German-Japanese Workshop that will be held in Japan in due time. ●



Figure 2:
Scientific Program



Figure 3:
Sightseeing walk through Dresden
passing Semper Opera House



Figure 2:
At the GAMM-Meeting in Munich 2018



Figure 5:
Trip to the winery “Schloss Wackerbarth”

Figure 4:
Workshop Banquet

The JACM is a union of researchers and engineers working in the field of computational mechanics mainly in Japan. JACM is a loosely coupled umbrella organization covering 29 computational mechanics related societies in Japan through communication with e-mail and web page (<https://ja-cm.org/index-e.html>). The number of individual members is about 350. JACM members actively participate in the IACM activities.

In 2019, The JACM Computational Mechanics Awards which are the highest awards were presented to Profs. Hiroshi Okuda (UTokyo), Makoto Yamamoto (Tokyo Univ. Science) and Makoto Ohsaki (Kyoto Univ.). The JACM Fellows Awards were presented to Profs. Koji Fukagata (Keio Univ.), Yoshiaki Tamura (Toyo Univ.), Daisuke Ishihara (Kyushu Inst. Tech.) and Daisuke Tagami (Kyushu Univ.). The JACM Young Investigator Award were presented to Profs. Akinori Yamanaka (Tokyo Univ. of Agri. and Tech.), Hikaru Aono (Tokyo Univ. Science) and Shin-ichiro Sugimoto (Hachinohe Inst. Tech.).

The award ceremony was held in the 2019 JACM Annual meeting which was held in Taipei during the period of APCOM (Asian Pacific Congress on Computational Mechanics) in December 2019. The details of the 2019 JACM Annual Meeting will be reported in an upcoming issue of IACM Expressions. ●



(a)



(b)



(c)

Figure 1:

Computational Mechanics Award: (a) Prof. Hiroshi Okuda (UTokyo), (b) Prof. Makoto Yamamoto (Tokyo Univ. Science) and (c) Prof. Makoto Ohsaki (Kyoto Univ.)



(a)



(b)



(c)



(d)

Figure 2:

Fellows Award: (a) Prof. Koji Fukagata (Keio Univ.), (b) Prof. Yoshiaki Tamura (Toyo Univ.), (c) Prof. Daisuke Ishihara (Kyushu Inst. Tech.) and (d) Prof. Daisuke Tagami (Kyushu Univ.)



(a)



(b)



(c)

Figure 3:

JACM Award for Young Investigators in Computational Mechanics (a) Prof. Akinori Yamanaka (Tokyo Univ. of Agri. and Tech.), (b) Prof. Hikaru Aono (Tokyo Univ. Science) and (c) Prof. Shin-ichiro Sugimoto (Hachinohe Inst. Tech.)

- JSCES Winter School 2019 on Topology Optimization and its Application for Additive Manufacturing -

JSCES Winter School 2019 on Topology Optimization and its Application for Additive Manufacturing was held on February 27, 2019, at Morito Memorial Hall of Tokyo University of Science. This course aims to provide teaching of fundamentals and the trends of topology optimization with some applications related to additive manufacturing. In addition, the special lecture was carried out by a researcher on additive manufacturing. Totally 63 participants consisted of engineers, researchers and university students attended the course (Figure 1). The lecturers were Prof. Junji Kato (Nagoya University) (Figure 2) and Assoc. Prof. Kuniharu Ushijima (Tokyo University of Science) (Figure 3). ●

by: Junji Kato



Figure 1:
A view of a lecture in the winter school



Figure 2:
Prof. Junji Kato



Figure 3:
Prof. Kuniharu Ushijima

- JSCES Summer School 2019 on Nonlinear Finite Element Method for Elastoplastic Analysis -

A three-day course “JSCES Summer School 2019 on Nonlinear Finite Element Method for Elastoplastic Analysis” was held during September 10-12, 2019, at Faculty of Science and Engineering (Korakuen Campus), Chuo University (Figure 4). The course has been hosted by JSCES since 2013, and held consecutively every year (2013 in Tokyo, 2014 in Nagoya, 2015 and 2016 in Tokyo, 2017 in Osaka, 2018 and 2019 in Tokyo), aiming at supporting engineers and students for their improvement in higher expertise on nonlinear analysis for solids and structures. The course has been attended by about 60 to over 100 participants every year, including engineers engaged in a broad range of industries, as well as university and college students. The total of around 480 attendees have taken the course since 2013.

The topics of the course encompass the basics of constitutive theory and finite element technology for small and large deformations, as well as practical techniques for numerical implementation. The lecturers, Profs. Kenjiro Terada, Isao Saiki, Yuki Yamakawa (Tohoku Univ.), Tateki Ishii (National Institute of Technology, Kisarazu College), Mao Kurumatani (Ibaraki Univ.), and Kazumi Matsui (Yokohama National Univ.) delivered lively lectures (Figure 5). After the lectures, an exchange meeting was held to facilitate communication and discussion among the participants and lecturers (Figure 6). ●

by: Yuki Yamakawa



Figure 4:
JSCES Summer School 2019



Figure 5:
Prof. Kenjiro Terada

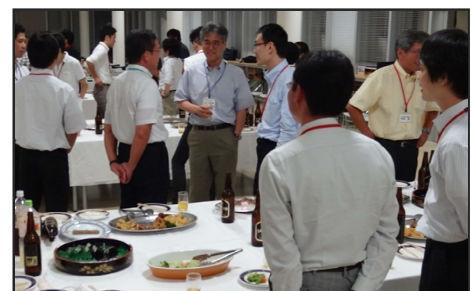


Figure 6:
Exchange meeting after the course

- JSCES Summer Camp for Students 2019 -

The summer camp for students 2019, a successful series hosted by JSCES from 2013, was held during September 14-15, 2019. This year, 23 students from various universities throughout Japan gathered in Nagatoro, which is a scenic town in the mountains of Saitama Prefecture (*Figure 7*). During this camp, 12 students presented their ongoing researches, and five keynote speakers including a student entrepreneur, Mr. Ihara (RICOS: Research Institute for Computational Science Co. Ltd), gave talks on their research experiences in universities, national laboratories and industry (*Figure 8*). The best presentation awards were given to two students (Mr. Minamite and Mr. Kanazawa) from Prof. Yamada, the President of JSCES (*Figure 9*). Attendees enjoyed a barbeque dinner after the lecture meeting and built good relationships through communication in a relaxed atmosphere. ●

by: Naoto Mitsume



Figure 7:
Attendees of Summer Camp 2019



Figure 8:
Mr. Ihara from RICOS, one of five keynote speakers



Figure 9:
Best presentation awards: (left) Mr. Minamite & (right) Mr. Kanazawa with Prof. Yamada

- Study Group on Uncertainty Modeling and Simulation -

This study group was launched in 2015 as one of the study groups in JSCES, aiming to investigate academic approaches toward uncertainty modeling and simulation. The group has been actively managed by 25 or more members including Chairperson, Naoki Takano (Keio University), and Vice-Chairpersons, Tetsuya Matsuda (University of Tsukuba) and two others from the industry. The members are mainly engineers or researchers in companies such as automotive manufacturers, construction companies and software vendors, and some members are from governmental research institutes or universities.

In the study group, workshops on various topics associated with uncertainty modeling/simulation and V&V had been held several times a year. And this year, seminars open to the public have been held twice to spread knowledge obtained by the group's activities (*Figure 10*). Moreover, based on such activities, we have been organizing a minisymposium in the annual conference of JSCES every year. Also, we have already organized some minisymposia at international conferences such as WCCM2016 in Seoul and COMPSAFE2017 in Chengdu, and will organize minisymposia at the upcoming COMPSAFE2020 in Kobe and WCCM-2020 in Paris. Currently, the members continue to work actively especially in industrial-academic collaborative working groups formed in the study group in 2019, which are specialized in uncertainty modeling/simulation methods for quenching of steel, 3D additive manufacturing, and the stochastic finite element method. ●

by: Tetsuya Matsuda & Naoki Takano

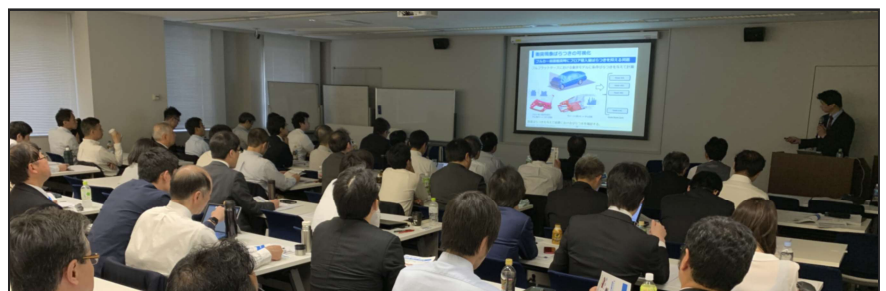


Figure 10:
Seminar on uncertainty modeling and simulation

MINISYMPOSIUM GIMC (Italian Group of Computational Mechanics) At the AIMETA Congress, Rome 15-19 September 2019



The AIMETA Computational Mechanics Group (GIMC) is pleased to announce that the minisymposium GIMC, held during the AIMETA Congress, in Rome on September 15-19 2019, was very successful and had a large turnout:

- 30 presentations and more than 70 participants, from Italian and foreign Universities;
- A special session devoted to the presentation of the PhD theses in Computational Mechanics winner of the GIMC award;
- A special session devoted to young researchers in which the best presentation has been awarded.



GIMC Best PhD Thesis Award

The GIMC Best PhD Thesis Awards committee, composed by **Loredana Contrafatto** (Università di Catania), **Massimiliano Cremonesi** (Politecnico di Milano), and **Giovanni Formica** (Università di Roma Tre), selected the following thesis defended during the 2018 year:

- **Dr. Domenico Magisano**, Università della Calabria, "*Solid-shell finite element and isogeometric models for nonlinear analysis and design of elastic shells using Newton, Koiter and Koiter-Newton solution strategies*" for the Computational Solid Mechanics Award
- **Dr. Elena Gaburro**, Università di Trento, "*Well balanced Arbitrary-Lagrangian-Eulerian Finite Volume schemes on moving nonconforming meshes for non-conservative Hyperbolic systems*" for the Computational Fluid Mechanics Award.

GIMC Best Presentation Award reserved to Young Researchers

The committee, composed by **Elena Benvenuti** (Università di Ferrara), **Stefano de Miranda** (Università di Bologna), **Giovanni Garcea** (Università della Calabria), **Sonia Marfia** (Università di Roma Tre), **Anna Pandolfi** (Politecnico di Milano) and **Giulio Ventura** (Politecnico di Torino), awarded the following young researchers for the best presentation:

- **Dr. Paolo Di Re**, Università della Calabria, "*Enhanced beam formulations with cross-section warping under large displacements*"
- **Dr. Francesca Fantoni**, Università di Brescia, "*Predicting the constitutive response of heterogeneous materials via machine learning*". ●

KSCM Spring Workshop & Award Ceremony 2019

The Korean Society for Computational Mechanics (KSCM) Spring workshop was held in the Coral room at the Millennium Seoul Hilton Hotel on 9 May 2019. Professor **Soo-Won Chae** at Korea University was awarded the KSCM medal, and Professors **Maenghyo Cho** at Seoul National University and **Byungsoo Kim** at Choongnam National University were awarded the KSCM research excellence awards.



1(a)

Figure 1 (a, b & c):
Invited lectures by KSCM awardees



1(b)



1(c)

After the award ceremony, they delivered invited lectures. The KSCM medal and awards are given by the KSCM to individual researchers in recognition of distinguished contributions to computational mechanics.

Besides, **Professors Sung Youb Kim** at UNIST, **Heung Soo Kim** at Dongguk University, and **Chohong Min** at Ewha Woman's University received the Young Scholar Awards.

Further information will be found at: <http://www.kscm-society.org/>. ●



Figure 2:
Group photo of awardees
and some participants.

During the past year the Israel Association for Computational Methods in Mechanics (IACMM) held two symposia. The **45th Israel Symposium on Computational Mechanics (ISCM-45)** was held in Oct 2018 at the Technion - Israel Institute of Technology, organized by Profs. Pinhas Bar-Yoseph and Sefi Givli. The interesting opening lecture was given by the international invited speaker Prof. John E. Dolbow from Duke University, USA, titled "Recent Advances in Computational Fracture Mechanics and Gradient-Based Damage Methods". *Figure 1* shows Prof. Dolbow lecturing. Prof. Adrian Lew from the Dept. of Mechanical Engineering, Stanford University, USA, gave a keynote lecture named "High-fidelity methods for brittle fracture propagation". The symposium included 10 other lectures, presented by practitioners and researchers from industry and academia. These included among others talks by Prof. Konstantin Volokh ("Material sink approach to fracture modeling"), and a tutorial on "Microstructural-based modelling of mechanical properties – Studying mechanical properties from the atomic scale", by Prof. Dan Mordechai, both from the Technion. Mr. Roman Kositski, a PhD student of Prof. Dan Mordechai from the Faculty of Mechanical Engineering, Technion was the winner of the ISCM-45 competition for the best presentation – the title of his talk was "The origin of the Hugoniot elastic limit spike and precursor decay in shocked body-centered cubic metals". *Figure 3* shows Mr. Kositski during his talk, and *Figure 4* is a group photo of the Invited speaker and the keynote speaker with the IACMM executive council.



Figure 1:
 Prof. Dolbow delivering the invited lecture of the ISCM-45, Oct 2018, Technion, Haifa



Figure 2:
 Prof. Adrian Lew during his talk at ISCM-45

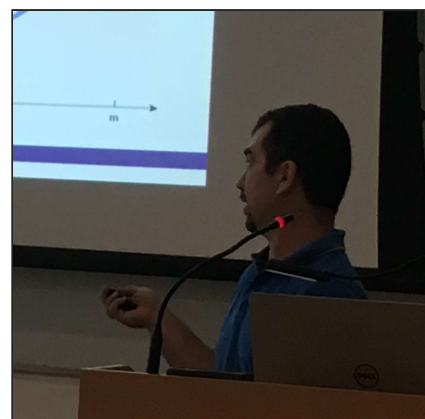


Figure 3:
 Mr. Kositski, the winner of the ISCM-45 competition for the best presentation, during his talk

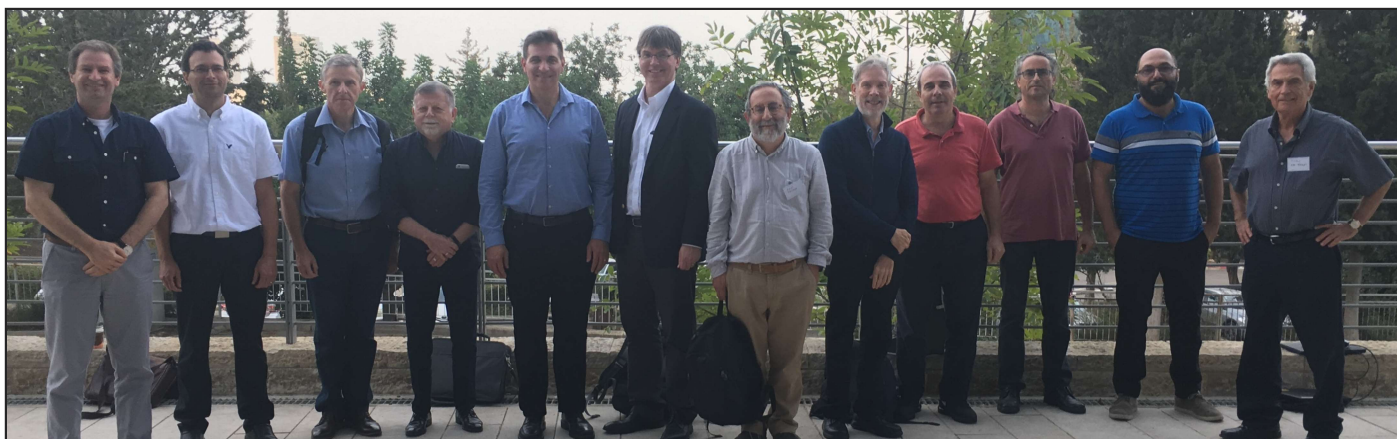


Figure 4:
 Group photo of IACMM executive council, international speaker, keynote speaker, organizers and tutorial speaker at ISCM-45, at the Technion. Left to Right: Z. Yosibash, S. Givli, S. Krylov, M. Engelman, A. Lew, J. Dolbow, A. Herszage, D. Givoli, I. Harari, J. Tal, D. Mordechai and P. Bar-Yoseph



Figure 5:
Prof. Wohlmuth delivers the invited lecture of the ISCM-46, March 2019, Tel-Aviv University



Figure 6:
Prof. Gyries delivers the tutorial lecture of the ISCM-46, March 2019, Tel-Aviv University



Figure 7:
Dr. Papadimitropoulos, the winner of the ISCM-46 competition for the best presentation, during his talk

The 46th IACMM Symposium was held in March 2019 at Tel Aviv University, organized by Profs. Slava Krylov and Isaac Harari. The delightful opening lecture was given by the international invited speaker Prof. Barbara Wohlmuth, from the Technical University of Munich, Germany, titled "Challenges and opportunities for numerical analysis in simulation technology". Figure 5 shows Prof. Wohlmuth lecturing. Seven additional presentations were given at ISCM-46, followed by a tutorial on "Deep learning basis" by Prof. Raja Gyries from Tel Aviv University (Figure 6 shows Prof. Gyries during his tutorial). The presentation by Dr. Symeon Papadimitropoulos, a PD working with Prof. Givoli at the Technion, was elected as the best presentation at ISCM-46, titled "Imaging in three-dimensional waveguides with partial aperture data". Figure 7 shows Dr. Papadimitropoulos during his talk and Figure 8 is a group photo of the Invited speaker with the IACMM executive council at the festive dinner held following ISCM-46.

The first prize winner of the best presentation at ISCMs in 2018, Mr. Roman Kositski, and the second prize winner, Dr Yaniv Brick, received an IACMM certificate awarded by IACMM president Prof. Zohar Yosibash during the assembly meeting of IACMM held at ISCM-46 (Figure 9). ●

Figure 8:
Group photo of IACMM executive council, the international speaker, and tutorial presenter at ISCM-46, at the festive dinner in Tel-Aviv Left to Right: R. Gyries, S. Krylov, Z. Yosibash, D. Givoli, I. Harari, B. Wohlmuth, P. Bar-Yoseph and M. Engelman



Figure 9:
Mr. Kositski receiving the certificate on best presentations in 2018 from Prof. Yosibash (president of IACMM) during the General Assembly of the IACMM at ISCM-46



26th UAKCM Conference prizes

The 26th Conference of the UK Association for Computational Mechanics took place from the 10th to 12th of April in City, University of London. The conference was organised by Professor Roger Crouch, Dean of the School of Mathematics, Computer Science and Engineering.

Figure 1:
Group photo of
the 26th UAKCM
conference participants
at the Goldsmiths' Hall
in London



After a long deliberation, the conference organizers awarded three prizes:

- **Yuxuan Chen** from Cambridge University received the Mike Crisfield Prize for the paper *"A Multigrid Approach that is Robust with respect to Mesh Quality"*.
- **Andrei Shvarts** from the University of Glasgow received the prize to the best presentation by a post-doctoral researcher for the paper *"FEM implementation for Navier-Stokes equations for an incompressible steady flow using hierarchical basis functions"*.
- **Zhi Li** from Swansea University received the prize to the best presentation by a PhD student for the paper *"An unsymmetric solid-shell element for geometric nonlinear analysis"*.

From UKACM we want to congratulate all the winners!

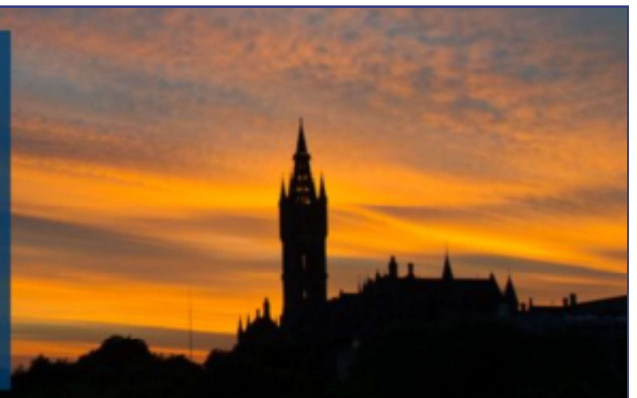
Computational modelling of Complex Materials across the Scales (CMCS)

The international ECCOMAS Thematic Conference "Computational Modelling of Complex Materials across the Scales (CMCS)" took place on 1-4 October 2019 in Glasgow.

The objective of CMCS was to elucidate cutting-edge developments in multi-scale computational modelling of complex materials, possessing distinct fine-scale structure and/or exhibiting coupled phenomena. Particular emphasis was on emergent coarse-scale behaviour due to the underlying fine-scale structure. CMCS thus focuses on both the (experimentally informed) modelling of complex fine-scale structural phenomena, and on their upscaling to coarser scales. CMCS gathered scientists from different disciplines working on scale-bridging challenges in complex materials to advance the field significantly.

The conference was chaired by Paul Steinmann (University of Glasgow, UK / University of Erlangen-Nuremberg, Germany), Andrew McBride (University of Glasgow, UK), Marc Geers (Eindhoven University of Technology, The Netherlands) and Julien Yvonnet (Université Paris-Est, France). ●

Computational modeling of
Complex Materials across
the Scales CMCS 2019



27th Conference of the UK Association for Computational Mechanics

The 27th UKACM Conference will take place on April 1-3, 2020 in Loughborough University. The conference will be organised by Dr Marco Discacciati, Lecturer at the Department of Mathematical Sciences and member of the UKACM Executive Committee.

As it is traditional in UKACM conferences, there will be a pre-conference School. This year the School will focus on virtual element methods, domain decomposition methods and reduced order modelling. The conference will start on Thursday 2nd April with three renowned speakers.

More details will be announced shortly in our website
www.ukacm.org.



2020 International Conference of the Engineering Mechanics Institute

The ASCE engineering mechanics institute international conference will take place on April 5-8, 2020. The conference is co-organized by Durham and Newcastle Universities and it is sponsored by UKACM. It will be hosted by Durham University, chaired by Professor John Brigham.

Submission of abstracts is already open and a number of minisymposia accepted in topics such as:

Bio-Mechanics/Materials, Computational Mechanics, Uncertainty Quantification and Data-Driven Science and Engineering, Design and Analysis of Next Generation Engineered Materials, Mechanics of Granular Materials and Coupled Systems, Mechanics of Materials, Mechanics of Structural Components and Systems and Structural Health Monitoring, Sustainability and Resiliency. ●





14th Conference of the French Structural Mechanics Association (CSMA), 13-17 May 2019, Giens, France

The 14th Conference of the French Structural Mechanics Association (CSMA) was held in Giens, in the south of France by 13-17 May 2019. CSMA conference is held every two years and is the major event for the French solids computational mechanics community. The 14th edition gathered 344 participants, 197 oral presentations, 28 posters and 5 parallel sessions. Distinguished plenary speakers included B. Sudret (ETH Zürich, Switzerland), A. Pandolfi (Politecnico di Milano, Italy), B. Leblé (Naval Group company, France), J.J. Marigo (Ecole Polytechnique, France), B. Cochelin (Ecole Centrale Marseille, France) and Yvon Maday (Sorbonne Université, France).

Events included a roundtable on data sciences in mechanics, a software session and the award ceremony for the best PhD theses in France on computational mechanics in 2018 and 2019. The topical sessions included:



- Statics and dynamics of structures
- Numerical methods
- Models and behavior of materials
- Durability of structures
- Biomechanics and bio engineering
- Manufacturing processes
- Optimization
- Contact mechanics, interfaces

In addition, mini symposia have been organized on the following topics:

- Data driven computational mechanics
- Digital materials and multiscale modeling
- Additive manufacturing simulations
- Bridging experiments and simulations
- Discrete elements, granular materials.

More information about the congress can be found on the website
<https://csma2019.sciencesconf.org/?forward-action=index&forward-controller=index&lang=en> ●

Julien Yvonnet
President of the Scientific committee

Hamid Zahrouni
Chair

3rd CSMA Juniors Workshop



CCSMA Juniors, the section of young researchers (<40) of the French Computational Structural Mechanics Association (CSMA), organized last spring the 3rd edition of its annual workshop. It took place in the beautiful Porquerolles Island (French Riviera) on 11-13 May 2019, and was connected with the 14th National CSMA Congress organized nearby in the Giens peninsula from May 13, 2019. It gathered about 60 participants (PhD students, post-docs, as well as junior researchers with permanent position), and it was a great success.

As usual, the workshop was a privileged place for scientific exchanges between the young generation of CSMA, with several social events. Several useful and unique activities with unconventional formats were also proposed such as:

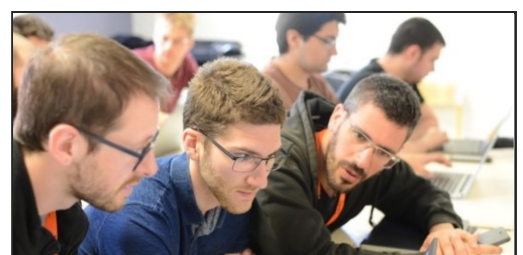
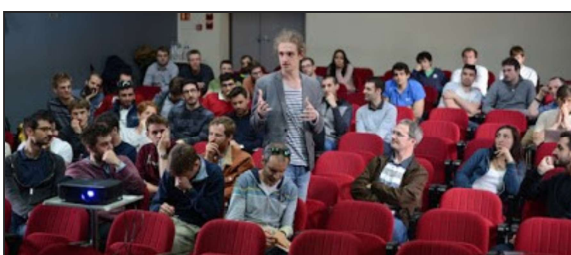
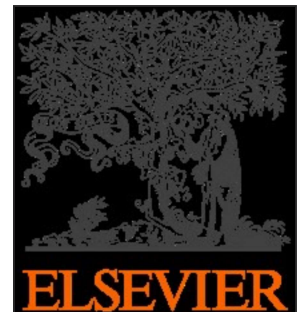
- a set of short courses (by and for young scientists) on the topics of the CSMA Congress mini-symposia, including both theoretical and practical parts with numerical implementation;
- a brainstorming session on data science, with a preliminary course on the topic;
- a session with short (180 s) and theatrical talks;
- a coding competition.

The 2019 CSMA Juniors Workshop was sponsored by CSMA, Elsevier, and EDF (French electricity company). The workshop organizers warmly thank these sponsors for their support.

For more information on activities of the CSMA Juniors section, which constitute an evidence of the dynamism of the CSMA association, please visit:

<http://csma.asso.univ-lorraine.fr/csma-juniors/> ●

Ludovic CHAMOIN
President of the CSMA Juniors Committee



USACM Thematic Conference: Modeling and Simulation of the Mechanics of Nanoscale Materials

The USACM Thematic Conference on Recent Advances in the Modeling and Simulation of the Mechanics of Nanoscale Materials, was held August 21-23, 2019 in the Singh Center for Nanotechnology of the University of Pennsylvania and sponsored by the USACM Thrust Area in Nanotechnology and Lower Scale Phenomena. The Penn Institute for Computational Sciences and National Science Foundation also provided support. There were 31 invited speakers, and a total of 64 participants. 20 posters were presented by graduate student and postdoctoral attendees. The successful workshop was organized by Celia Reina and David Srolovitz from the University of Pennsylvania, Long-Qing Chen from Pennsylvania State University, and Vasily Bulatov from Lawrence Livermore National Laboratory.

The workshop gathered experts at the forefront of the modeling and simulation of the mechanics of nanoscale materials, while ensuring a diversity of computational techniques and participants. Approaches discussed included (but were not be limited to) electronic structure calculations, atomistic modeling, continuum approaches for microstructure evolution and bridging techniques. These technique oriented presentations were complemented by a diverse set of applications. Session were held on First Principle Calculations and Quantum Properties, Plasticity, Defects, Grain Boundaries and Interfaces, Mechanics of Materials, Phase Field Models, and Scale Bridging.

The speakers at the workshop were Vikram Gavini, Amartya Banerjee, Mauricio Ponga, David Rodney, Eugen Rabkin, John Bassani, David McDowell, Michael Ortiz, Emmanuel Clouet, Jaime Marian, Anter El-Azab, Yash Kulkarni, Nikhil Admal, Brandon Runnels, Garritt Tucker, Tim Rupert, Jun Lou, Mitra Taheri, Ryan Elliot, Prashant Purohit, Andrej Kosmrij, Pradeep Sharma, Kaushik Dayal, Pedro Ponte-Castanada, Peter Voorhees, Katsuyo Thornton, Martin Diehl, Jarek Knap, Yuri Mishin, Xin Yan, Dan Mordehai,

and Andrea Liu. Further details about the conference program can be found in the conference webpage -

<http://nanomaterials2019.usacm.org>

An active student poster session was held on the first evening of the workshop and was attended by all workshop participants. There were a total of 20 posters presented. ●



Figure 1:
Attendees at Recent Advances in the Modeling and Simulation of Nanoscale Materials, Philadelphia, PA, August 20-22, 2019

USACM Upcoming Events *further details at usacm.org*

- **Workshop on Experimental and Computational Fracture Mechanics: Validating Peridynamics and Phase Field Models**, February 26-28, 2020; Baton Rouge, Louisiana; <http://wfm2020.usacm.org/>
- **Meshfree and Novel Finite Elements with Applications**, September 27-29, 2020; Berkeley, California; <http://mfem2020.usacm.org>
- **Isogeometric Analysis 2020**, October 18-21, 2010; Banff, Canada; <http://iga2020.usacm.org> ●

15th U.S. National Congress on Computational Mechanics

The 15th U.S. National Congress on Computational Mechanics (USNCCM15) was held July 28 - August 1, 2019 at the JW Marriott in Austin Texas. Led by co-chairs John Foster, Tan Bui-Thanh and the local organizing committee from the Oden Institute for Computational Sciences and Engineering at the University of Texas, the congress had several highlights, beginning with Texas singer-songwriter Gary P. Nunn entertaining attendees at the Opening Reception. The congress was also pleased to honor Professor Mary F. Wheeler for her long and distinguished career in subsurface modeling. Three minisymposia were dedicated to Professor Wheeler and she was a guest speaker at the Women's Networking Event.

During the opening ceremony, the 2019 USACM Awards were presented as follows:

1. **John Von Neumann Medal:** Michael Ortiz, *California Institute of Technology*
2. **The Belytschko Medal:** Romesh Batra, *Virginia Institute of Technology*
3. **Thomas J.R. Hughes Medal:** John Shadid, *Sandia National Laboratories and the University of New Mexico*
4. **J. Tinsley Oden Medal:** Suvranu De, *Rensselaer Polytechnic Institute*
5. **Gallagher Young Investigator Medal:** Ming-Chen Hsu, *Iowa State University*
6. **USACM Fellows:**
 - a. Krishna Garikipati, *University of Michigan*
 - b. Lori Graham-Brady, *Johns Hopkins University*
 - c. Yongjie Jessica Zhang, *Carnegie Mellon University*

Plenary speakers for the congress were Karen Willcox, *Oden Institute, UT-Austin*, Carlos Armando Duarte, *University of Illinois at Urbana-Champaign*, Mary F. Wheeler, *Oden Institute, UT-Austin* and Travis Oliphant, founder and head of Quansight.

Semi-Plenary speakers were Stewart Silling, *Sandia National Laboratories*, Victor Calos, *Curtin University*; Caglar Oskay, *Vanderbilt University*; Ellad Tadmor, *University of Minnesota*. A new feature of the US National Congress was the Special Young Investigator Semi-Plenary Speakers: Miguel Bessa, *Delft University* and Michael Tupak, *Sandia National Laboratories*.

The Plenary and Semi-Plenary talks were recorded and are to be available for viewing at: <https://www.youtube.com/channel/UCNZ0Lojf6ww8cKspMGdT47g/>.

A student poster competition was held during the afternoon session of the second day. Six winners were announced at the congress banquet as follows:...

- Angran Li, *Carnegie Mellon University*
- Jonathan Russ, *Columbia University*
- Nicole Nellesen, *RWTH Aachen*
- Berkin Dortdivanlioglu, *Stanford University*
- Farzaneh Mousavi, *University of Nebraska-Lincoln*
- Hugh Carson, *MIT*

Over 1000 were in attendance at the congress, with 75 participating in 5 pre-congress short courses. The congress also featured the Women's Networking Event, held in support of and for mentoring women in research. The next congress will be held July 25-29, 2021 in Chicago, Illinois. ●



Figure 2:
Professor Mary Wheeler
addressing the participants
of the Women's
Networking Event



Figure 3:
USACM President,
John Dolbow (center) and
2019 USACM Awardees

Figure 4:
Poster session at
USNCCM15



SEMNI and APMTAC met this July for their biannual conference

The Spanish and Portuguese associations, SEMNI and APMTAC, celebrate this July their biannual conference in Guimarães, Portugal. All the relevant information, along with the program of the congress, is available at <http://www.cmn2019.pt>.

Figure 1:
A picture of the
opening session
of the conference



Nearly 100 Spanish researchers joined the Portuguese community in Guimarães.

The conference was a great success both from the scientific as well as social points of view. ●

Figure 3:
Prof. Paulo Lourenço,
Glaucio H. Paulino and
Oscar Lopez-Pamies
during the plenary lecture of
Prof. Paulino



SEMNI awards 2019

SEMNI has awarded its annual prizes during its last meeting of the executive board, held in Barcelona the last March 29th, 2019. The awardees will receive their prizes during the gala dinner ceremony of the joint Spanish-Portuguese Conference on Numerical Methods, CMN, to be held in Guimarães, Portugal the next July 1-3rd, 2019.

The list of awardees is the following:

SEMNI award to the best Ph.D. thesis in the field of numerical methods:

The committee, formed by profs. I. Romero (president), M. Arroyo, S. Badía, L. Cueto-Felgueroso and E. Reina, granted the prize to:

- **Dr. Aranu Pont**, for the thesis "Numerical Simulation of Aeroacoustics using the Variational Multiscale Method. Application to the problem of human phonation" advised by Ramon Codina and Joan Baiges (Universitat Politècnica de Catalunya). This thesis has represented SEMNI for the ECCOMAS award 2019.
- **Dr. Miguel Herráez** (ex aequo), for the thesis "Computational Micromechanics Models for Damage and Fracture of Fiber-Reinforced Polymers" advised by Carlos González and Claudio Lopes (Universidad Politécnica de Madrid).

Juan C. Simó award 2019:

SEMNI's prize to young researchers commemorates the legacy of the late prof. Juan C. Simó in the field of numerical methods. The committee was formed in this occasion by profs. P. Díez (president), M. Doblaré, S. Idelsohn, D. Peric and J. P. Moitinho de Almeida. In this occasion, the awardee is:

- **Prof. José Reinoso**, from the University of Seville. The committee highlighted his contributions to the field of non-linear solid mechanics, particularly in composite material modeling and simulation.

SEMNI O. C. Zienkiewicz award

The highest distinction provided biannually by SEMNI to personalities in the field of numerical methods in engineering is the O. C. Zienkiewicz prize. In this occasion, the award goes to:

- **Prof. Manuel Doblaré**, from the University of Zaragoza. Prof. Manuel Doblaré is a member of the Spanish Royal Academy of Engineering and a renowned specialist in the field of numerical methods, biomechanics and mechanobiology. Prof. Doblaré will receive a diploma and a plaque during the gala dinner of the next Conference on Numerical Methods, CMN, to be held in Guimarães, Portugal, next July 1-3rd, 2019.

Traditionally, SEMNI O. C. Zienkiewicz awardees deliver a plenary lecture during this same conference. In this case, the conference is entitled *From Data-Driven modeling to Physically-Constrained Deep Learning in Predictive Continuum Physics*, where he will overview the results of his research in the field. ●

Figure 3:
*Prof. Doblaré (left) receiving
his SEMNI O. C. Zienkiewicz
award 2019*



PCM-CMM 2019 The 4th Polish Congress of Mechanics &

23rd International Conference on Computer Methods in Mechanics

On September 8-12 2019, a joint scientific event including the 4th Polish Congress of Mechanics (PCM) and the 23rd International Conference on Computer Methods in Mechanics (PCM-CMM 2019) was held in Cracow in Auditorium Maximum, the congress centre of the Jagiellonian University. The PCM-CMM 2019 Congress was co-organized by the Polish Society of Theoretical and Applied Mechanics and Polish Association for Computational Mechanics (PACM). The congress was organized under auspices of the European Community on Computational Methods in Applied Sciences (ECCOMAS) as the ECCOMAS Special Interest Conference.

The 4th Polish Congress of Mechanics (PCM) continues the tradition of scientific meetings on mechanics, initiated around 12 years ago. The Congress was aimed to present the current state of the art research in all disciplines of mechanics, solid and fluid mechanics, computational mechanics, applied mathematics and physics, as well as structural mechanics and mechanical engineering. This and previous editions of the PCM congress were organized jointly with the CMM conferences. The CMM conference series is devoted to numerical methods and their applications to the study of the various phenomena in mechanics. The CMM conferences are organized regularly every two years, starting in 1973.

Prof. Michał Kleiber (Polish Academy of Sciences, President of ECCOMAS) acted as the Congress Chairman, Prof. Włodzimierz Kurnik (Warsaw University of Technology) as the Congress Vice-President, the Honorary Chairmanship was bestowed upon Prof. Witold Gutkowski (Polish Academy of Sciences). The Scientific Committee was chaired by Prof. Tadeusz Burczyński (Institute of Fundamental Technological Research of Polish Academy of Sciences) and the Organizing Committee was chaired by Prof. Błażej Skoczeń from Cracow University of Technology. Andrzej Duda, President of the Republic of Poland has kindly granted Honorary Patronage to the Congress, and Jarosław Gowin, Minister of Science and Higher Education, has chaired the Congress Honorary Committee. Both President Andrzej Duda and Minister Jarosław Gowin attended and delivered speeches at the opening ceremony.

The scientific programme of the PCM-CMM 2019 Congress was composed of 12 plenary lectures, 4 thematic sessions and 22 mini-symposia. There were 550 participants from Poland and 27 countries from Europe, Asia and North America. The following distinguished scientists held the interesting plenary lectures on current research topics:

- **Leszek Demkowicz**, USA, *Progress Report on the DPG Method*
- **Fionn Dunne**, Great Britain, *Microstructurally-Sensitive Fatigue Crack Nucleation and Growth: Dislocation Configurational Energy and Crystal Plasticity Approaches*
- **Thomas J.R. Hughes**, USA, *The Isogeometric Approach to Analysis*
- **Tomasz Lewiński**, Poland, *Least Weight Structures and Least Compliant Bodies. Optimal Layout Problems and Recovery of Underlying Microstructure*
- **Shaker Meguid**, Canada, *Multiscale Modeling of Multifunctional Nanocomposites*



Figure 1:
Distinguished guests at the opening ceremony: third from left Andrzej Duda, President of the Republic of Poland, fourth from left Jarosław Gowin, Minister of Science and Higher Education, first from right Michał Kleiber, President of ECCOMAS

Opportunities and Challenges

- **Andreas Menzel**, Germany, *Electro-Viscoelasticity of Dielectric Elastomers – Experiment, Modelling and Simulation*
- **Bernd R. Noack**, Germany, *Turbulence Control - Better, Faster and Easier with Machine Learning*
- **Jerzy Pamin**, Poland, *Numerical Simulation of Material Instabilities*
- **Henryk Petryk**, Poland, *On Microstructural Length Scales in Single Crystals*
- **Franz G. Rammerstorfer**, Austria, *Some Oddities in Plate and Shell Buckling*
- **Meir Shillor**, USA, *Recent Results on Dynamic Contact, Friction, Heat, Exchange, and Debonding*
- **Marek Stankiewicz**, Poland, *Synchrotron SOLARIS - Large Research Infrastructure and Its Mechanical Challenges*

It has become a tradition that during the CMM conferences the O.C.Zienkiewicz Medal Awarding Ceremony takes place to honour outstanding researchers in the field of computational mechanics. This year's awarding ceremony was held during the congress opening. The 2019 laureates of the O.C. Zienkiewicz Medal are:

- **Prof. Tomasz Lewiński** in the category for the whole of activity,
- **Prof. Jerzy Pamin** in the category for the whole of activity,
- **Prof. Thomas J.R. Hughes** in the category for foreign scientists of particular merit for the development of computational mechanics in Poland.

The awards were presented by Prof. Michał Kleiber (Commander of the Medal Chapter) and Prof. Tadeusz Burczyński (Chancellor of the Medal Chapter), during the ceremony conducted by Prof. Jerzy Rojek (President of PACM).

During the conference there was also held the Jan Schmelter competition for young scientists. Jury of the competition led by Prof. Waldemar Rachowicz (Cracow University of Technology) awarded three prizes to the following young scientists:

- 1st place: **Nicola A. Nodargi** – University of Rome Tor Vergata
 - 2nd place: **Tomasz Schlieter** – Silesian University of Technology
 - 3rd place: **Witold Ogierman** – Silesian University of Technology
- and one recognition award to **Paulina Świątkiewicz** from Lodz University of Technology.

The General Assembly of PACM was held during the conference. At the meeting, PACM president Jerzy Rojek presented a report on PACM activities and achievements during the last term 2017-2019. The report was accepted unanimously. Prof. Jerzy Rojek was elected president of PACM for the next term 2019-2021.

The PCM-CMM 2019 congress was a successful, well-organized scientific event. More details on PCM-CMM 2019 congress can be found at the conference web site: <https://pcm-cmm2019.com/en/>. The next, 24th International Conference on Computer Methods in Mechanics will be organized by the West Pomeranian University of Technology Szczecin in September 2021. Prof. Ryszard Buczkowski will chair the organizing committee. The next 5th Polish Congress of Mechanics will be held in Gliwice (Upper Silesia) in 2023. ●



Figure 2:
*Andrzej Duda,
President of the
Republic of Poland,
delivers a speech at
the opening ceremony*

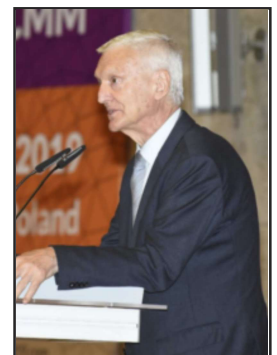


Figure 3:
*Michał Kleiber,
President of
ECCOMAS, delivers
a speech at the
opening ceremony*



Figure 4:
*Awarding Ceremony of the O.C. Zienkiewicz Medal.
From left to right:
Thomas J.R. Hughes, Jerzy Pamin, Tomasz Lewiński – recipients of
Medal, Jerzy Rojek – President of PACM,
Michał Kleiber – Commander of the Medal Chapter,
Tadeusz Burczyński – Chancellor of the Medal Chapter*

ENIEF 2019
XXIV Congress on Numerical Methods
and their Applications
Santa Fe, Argentina
5 - 7 November 2019

The XXIV Congress on Numerical Methods and their Applications (ENIEF 2019) took place from November 5 through November 7, 2019, at the city of Santa Fe, Argentina. This new edition of the annual AMCA Congresses was organized by the Research Centre on Computational Methods (CIMEC), dependent on the National University of the Littoral (UNL) and the Argentine Council for Research in Science and Technology (CONICET), together with the Argentine Association of Computational Mechanics (AMCA).

The Organizing Committee included Prof. Alberto Cardona (chairman), Prof. Sergio Idelsohn (honorary chairman), Prof. Pablo Kler and Prof. Santiago Márquez Damián (co-chairmen). The Scientific Committee was chaired by Prof. Mario Storti, with Prof. Luciano Garelli and Prof. Juan Marcelo Giménez as co-chairmen.

The Congress hosted seven invited lectures by Prof. Rainald Löhner (George Mason University, USA), Prof. Jaime Klapp (National Institute for Nuclear Research, Mexico), Prof. Adrian Lew, (Department of Mechanical Engineering, Stanford University, USA), Prof. Marcela Cruchaga (University of Santiago de Chile, Chile), Prof. Roberto Lamberts (Laboratory for Energy Efficiency in Buildings, Federal University of Santa Catarina, Brazil), Prof. Luis Caffarelli (University of Texas at Austin, USA), and Prof. Mariano Vázquez (Barcelona Supercomputing Center and ELEM Biotech, Spain).

The Congress was held at Estación Belgrano Conventions Center, a renewed former train station located at an iconic place in Santa Fe, and was attended by 300 researchers and students from Argentina, Brazil, Chile, Colombia, Uruguay, Costa Rica, Ecuador, Germany and Spain. Full-length papers were submitted to a review process prior to publication. Accepted papers have been published in proceedings which are openly available at the website <http://www.amcaonline.org.ar/mcamca>

A special session was devoted to undergraduate students, with awards for the best posters, that were granted to:

1. **Pablo N. Wierna**, from the Applied Mechanics Research and Development Group (GIDMA) of the National Technological University at Cordoba, Argentina.
2. **Tomás Leschiutta**, from the National Technological University (UTN) at Santa Fe, Argentina.
3. **Facundo Castañón**, from the Applied Multiphysics Research Group (GIMAP) of the National Technological University at Bahia Blanca, Argentina.

Figure 1:

*Opening Ceremony,
from left to right:*

*Prof. Alberto Cardona (chair
of the congress),
Prof. Enrique Mammarella
(Rector of UNL),
and Víctor Fachinotti
(president of AMCA)*



Figure 2:

Welcome cocktail on a boat through Setúbal lagoon





Figure 3:
All the participants of the conference at Estación Belgrano main entry

During the congress dinner, Prof. Luis Caffarelli received the AMCA International Scientific Trajectory Award which was already announced last year.

The Congress also included other activities like the VIII Meeting of OpenFOAM users and the special session to honor Prof. Victorio Sonzogni (former president of AMCA) for his retirement. ●



Figure 4:
Special session to honor Prof. Victorio Sonzogni



Figure 5:
Prof. Luis Caffarelli receiving the AMCA Award from Prof. Sergio Idelsohn

MECOM 2020
XXXVII Argentine Congress
for Computational Mechanics
November 3-5, 2020
Resistencia, Chaco, Argentina

CALL FOR PAPERS

The Argentine Association for Computational Mechanics (AMCA) announces the XXXVII Argentine Congress for Computational Mechanics (MECOM 2020), which will be held at Resistencia, Argentina, organized by the Faculty of Engineering of the National University of the NorthEast (UNNE) and AMCA.
<http://amcaonline.org.ar/mecom2020> ●



conference diary planner

18 - 21 Dec 2019	APCOM 2019 - 7th Asian Pacific Congress on Computational Mechanics <i>Venue:</i> Taipei, Taiwan <i>Contact:</i> http://www.apcom2019.org/
26 - 28 Feb 2020	USACM Thematic Conference - Large Scale Structural Systems and Optimal Design <i>Venue:</i> Baton Rouge, LA, USA <i>Contact:</i> http://wfm2020.usacm.org/organizers
4 - 6 March 2020	1st BICTAM-CISM Symposium on Dispersed Multiphase Flows: from Measuring to Modeling <i>Venue:</i> Beijing, China <i>Contact:</i> http://158.110.32.35/BICTAM-CISM
8 - 11 March 2020	COMSAFE 2020 - Computational Engineering & Science for Safety & Environmental Problems <i>Venue:</i> Kobe, Japan <i>Contact:</i> https://www.compsafe2020.org/
15 - 18 March 2020	IUTAM Special Event: Fluid Mechanics in the Spirit of G.K. Batchelor <i>Venue:</i> Cambridge, UK <i>Contact:</i> http://www.damtp.cam.ac.uk/events/
1 - 3 April 2020	2020 Conference of the UK Association for Computational Mechanics <i>Venue:</i> Loughborough University, UK <i>Contact:</i> http://ukacm.org/ukacm-conferences/
5 - 8 April 2020	EMI 2020-IC ASCE Engineering Mechanics Institute International Conference <i>Venue:</i> Durham, UK <i>Contact:</i> https://sites.durham.ac.uk/emi2020-ic/
9 - 11 June 2020	14th Int. Confonference on Computational Fluid Dynamics In the Oil & Gas, Metallurgical & Process Industries <i>Venue:</i> Trondheim, Norway <i>Contact:</i> https://www.sintef.no/cfd2020/
22 - 26 June 2020	ECCM19 - European Conference on Composite Materials <i>Venue:</i> Nantes, France <i>Contact:</i> www.eccm19.org
13 - 17 July 2020	BAIL 2020 - International Conference on Boundary and Interior Layers <i>Venue:</i> Buenos Aires, Argentina <i>Contact:</i> https://amcaonline.org.ar/
19 - 24 July 2020	ECCOMAS CONGRESS 2020 jointly organized with the WCCM XIV - 14th World Congress on Computational Mechanics (IACM) <i>Venue:</i> Paris, France <i>Contact:</i> http://www.eccomas.org/
23 - 28 Aug 2020	25th ICTAM - International Congress of Theoretical and Applied Mechanics <i>Venue:</i> Milan, Italy <i>Contact:</i> https://www.ictam2020.org/
16 - 18 Sept 2020	SAHC 2020 - International Conference on Structural Analysis of Historical Constructions <i>Venue:</i> Barcelona, Spain <i>Contact:</i> http://congress.cimne.com/SAHC2020/
27 - 29 Sept 2020	USACM Thematic Conference - Novel Methods in Computational Engineering and Sciences <i>Venue:</i> Berkeley, California <i>Contact:</i> http://mfem2020.usacm.org/
18 - 21 Oct 2020	USACM Thematic Conference - Isogeometric Analysis 2020 <i>Venue:</i> Banff, Canada <i>Contact:</i> http://iga2020.usacm.org/
19 - 21 Oct 2020	IGA2020 - Isogeometric Analysis 2020 <i>Venue:</i> Banff, Canada <i>Contact:</i> ruth@usacm.org
1 - 5 Nov 2020	International Conference on Multibody System Dynamics & Asian Conference on Multibody Dynamics 2020 <i>Venue:</i> New Delhi, India <i>Contact:</i> https://iutam.org/
2 - 6 Nov 2020	IUTAM Symposium on Computational fracture mechanics in multi-field problems <i>Venue:</i> Bad Honnef, Germany <i>Contact:</i> https://iutam.org/
3 - 5 Nov 2020	MECOM 2020 - XXXVII Argentine Congress for Computational Mechanics <i>Venue:</i> Resistencia, Argentina <i>Contact:</i> http://amcaonline.org.ar/mecom2020
17 - 21 Oct 2021	21st International Symposium on Finite Element Methods in Flow Problems <i>Venue:</i> Hangzhou, China <i>Contact:</i> https://iacm.info/scientific-events/fef/