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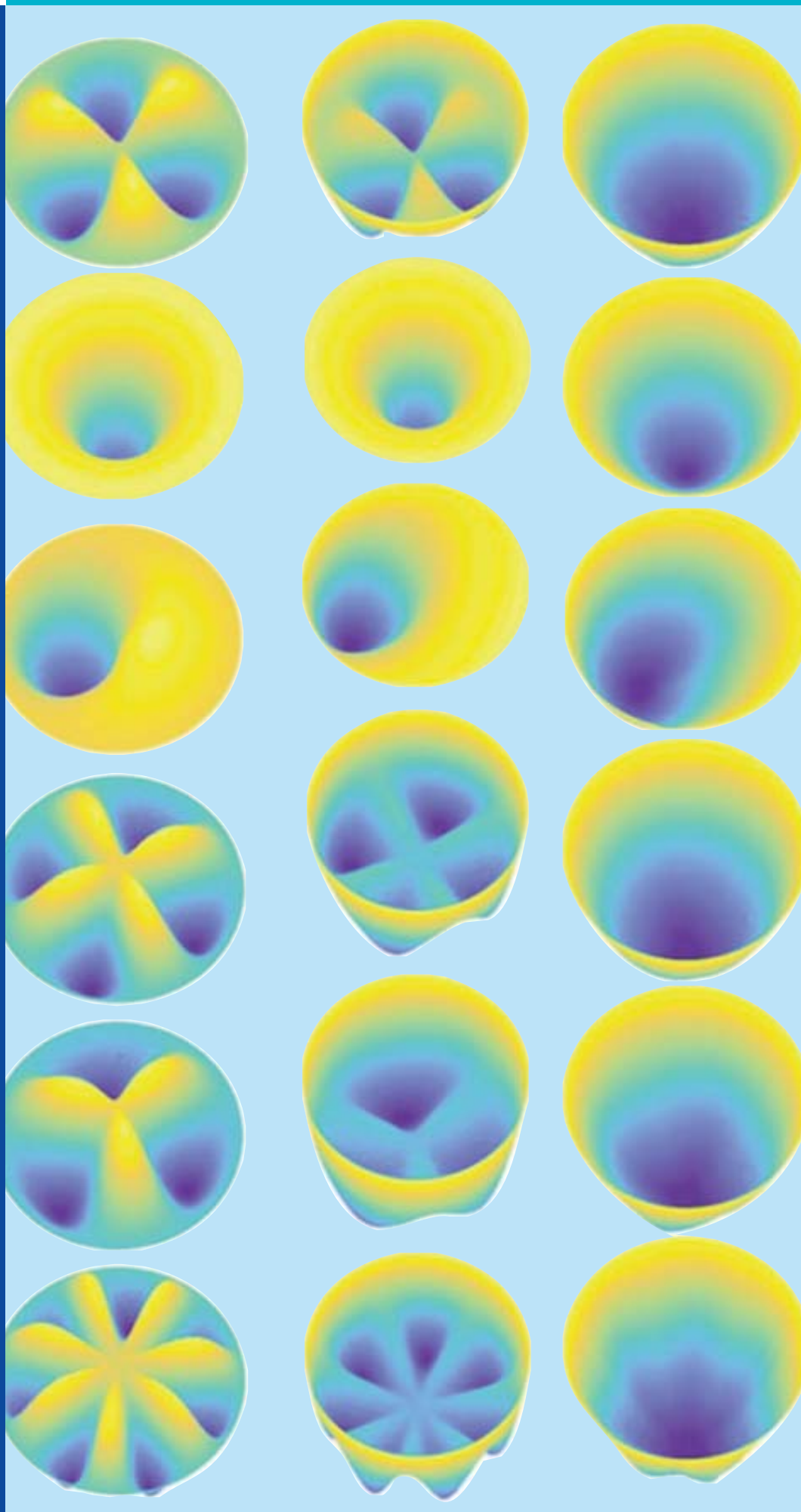

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contents

editorial

The three review articles published in this issue of Expressions deal with topics that are directly or indirectly related to multiscale computations. Indeed, simulation-based techniques rooted on the principles of computational multiscale methods are increasingly used to study mechanical and living systems accounting for the multiple physics, time scales and levels of spatial organization of the system under study.

But the possibility of multiscale computations go far beyond the classical fields of engineering mechanics. An example is the broad field of computational social sciences. For instance, the "tri-junction" between multiscale computations, bifurcation theory and social networks can be used for deriving a computational framework to systematically extract coarse-grained, emergent dynamical information from a social system by bridging detailed, agent-based models of social interactions on networks, with macroscopic, systems-level, continuum numerical analysis tools. (https://www.worldscientific.com/doi/abs/10.1142/S0218127410027945).

The application of numerical algorithms for predictive computations in particular fields of social sciences has recently had a high impact in the mass media via a disturbing proposal from the British mathematician Dr. Hannah Fry. After completing her PhD in computational fluid dynamics in early 2011, and a professional period as an aerodynamicist in the motorsport industry, Dr Fry began work on an interdisciplinary project in complexity sciences at University College London. Her current research focusses on discovering new connections between mathematically described systems and human interaction at the largest scale. In her recent publications and talks under the general and provocative title of the Mathematics of Love, Dr Fry shows algorithmic patterns in how we look for love, and gives her top three tips (verified by maths!) for finding that special someone [sic]. https://www.ted.com/speakers/hannah_fry .

If to the previously mentioned singular predictive methods of "social impact" we add virtual reality (VR) and augmented reality (AR) techniques, we can anticipate a revolution in the way we obtain, store, process and disseminate (or use) the information that results from multiscale computations in all types of technical and non-technical problems that affect human life. https://www.ted.com/topics/augmented+reality. For instance, new tools will be available soon that will allow us to master the use of VR and AR techniques for a variety of academic and industrial applications. Here, the possibility of creating and customizing "avatars" that will assist us in daily tasks is not anymore a so far away futuristic proposal. https://secondlife.com/

It is certainly debatable that this fanciful future will be a reality of practical value in the next coming years. What I am convinced is that the crossroad of the new non-standard simulation technologies and applications mentioned above will bring many opportunities for the broad field of computational mechanics. I recommend that we keep an open eye on these special simulation-based predictive techniques.

Many of us will soon meet in another successful IAMC event: the 13th World Congress on Computational Mechanics that will be held on 22-27 July 2018 in the city of New York. Over 3500 participants from all over the world will attend the gathering jointly organized with the 2nd Pan American Congress on Computational Mechanics. Indeed, the different events regularly promoted by the IACM in different countries (www.iacm.info) are unique occasions for meeting and interacting with colleagues from other world regions.

Eugenio Oñate
Editor of IACM Expressions

Multi-Scale Computational Simulation and Design of Photo-Deformable Structures

by
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Photo-responsive polymers (PRPs) can exhibit remarkable macroscopic deformations in response to light. Compared with conventional smart materials, PRPs have attractive features such as remote and wireless control, complex 3D deformation with a simple fabrication, and environmentally-friendly operation for actuation devices. Among those, azobenzene-containing liquid crystalline polymers (LCPs) can realize reversible deformation under ultraviolet (UV) or visible light irradiation. The origin of the photo-mechanical response is attributed to reversible photo-isomerization. As photons with adequate frequency are incident on the PRP, trans-state azobenzenes change their form into the cis-state. The photo-chemical process causes a phase transition of the liquid-crystalline state and an associated polymeric shape change. This complex photo-mechanical process has been applied to micro-mechanical devices such as light-driven motor, soft robotic arm, micro-pumps, etc. [1-3]. However, our current understanding of the opto-mechanical mechanism heavily relies on experimental measures. A comprehensive theoretical approach and scale-integrated computation are required to broaden the applicability of PRPs and to design complex deformations.

We developed a multi-scale computational model integrating quantum mechanics (QM), molecular dynamics (MD), and finite element method (FEM) simulation techniques. *Figure 1* shows how physical phenomena in each scale are bridged to systematically design the deformation of the photo-responsive material. The QM calculation provides the profile of the photo-isomerization ratio with respect to light intensity. From the MD simulation, we can obtain the microscopic polymeric conformation change and phase transition behavior. Then, we up-scaled the parameters with the aid of a nonlinear FEM model to examine the photo-bending behavior. The detailed computational approach and background theory in each scale are presented in the following paragraphs.

To predict the photo-isomerization ratio of the azobenzene group, the Stimulated Raman Adiabatic Passage (STIRAP) method was used [4]. The STIRAP method is based on solving the time-dependent Schrödinger equation with respect to each individual electronic state (Figure 2), and estimates the trans/cis ratio of the azobenzene molecule according to light intensity and polarization angle. The photo-chemical properties of

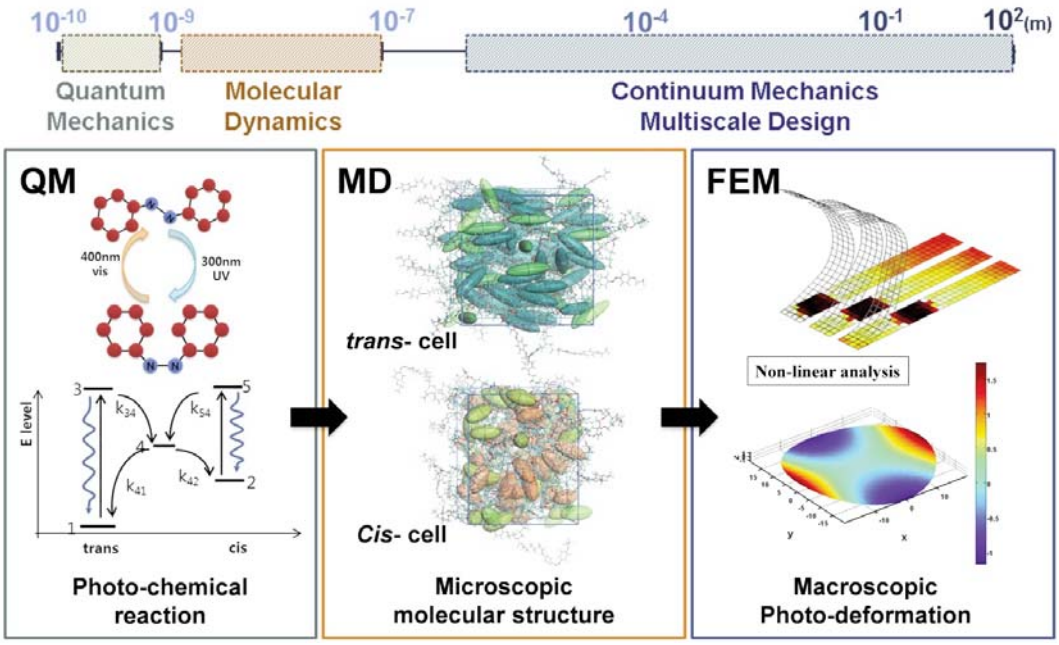


Figure 1: *Schematic of the multi-scale computational approach to analyze the photo-mechanical deformation of the PRP*

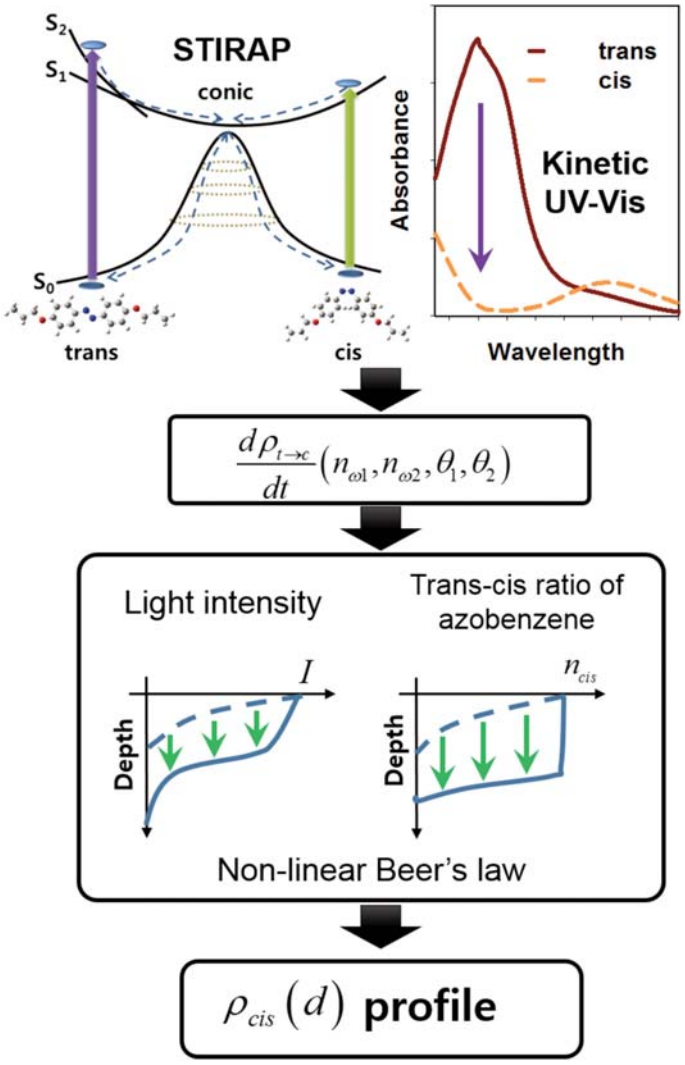
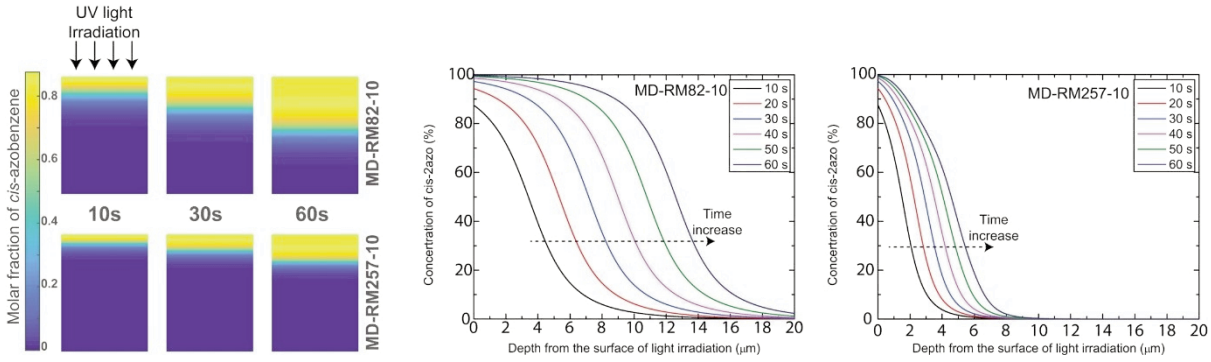


Figure 2:
Flowchart of STIRAP-Beer's law modeling, where pcis(d) indicates cis-population of azobenzene according to penetration depth d [4]

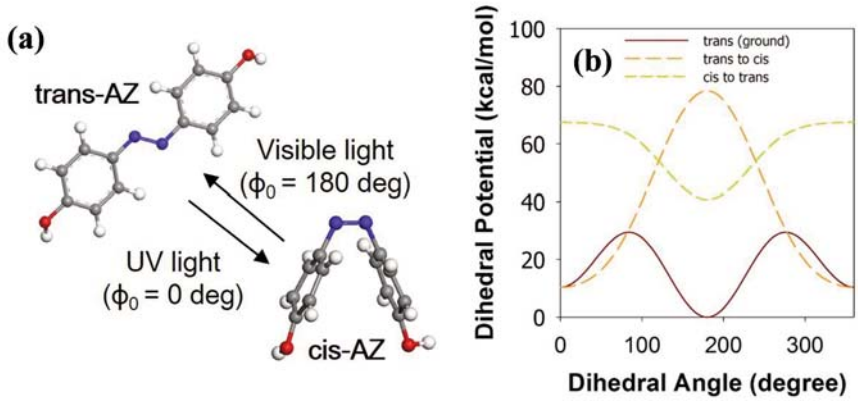
the azo-monomer (energy level, transition dipole moment, and vibrational frequency) were obtained from a density functional theory (DFT) calculation, and employed in the governing equation of the STIRAP formulation to reflect the characteristic tendency of the trans-cis transition among multiple electronic states. From the derived photo-isomerization ratio, the trans-cis conversion of the entire LCP domain was calculated by incorporating this data into non-linear Beer's law. When light penetrates into the LCP, the intensity of the light decays with respect to the thickness of the sample. Moreover, the trans-cis conversion of the azobenzene changes the light absorption efficiency of the PRP. Therefore, effective intensity of the light within the PRP is changing through the time evolution. Because both light absorbance and photo-isomerization simultaneously influence each other, a feedback algorithm was constructed to track the time-evolutional change of both light intensity and cis-population *(Figure 2)*. As a result, we predicted the profile of isomerization ratio along light penetration depth with two different types of LC hosts *(Figure 3)* [5], and the calculated data was applied to the MD simulation.



MD simulation was utilized to observe the microstructural evolution of the bulk polymer network in response to light. While the QM calculation accounts for the electronic state of the azo-containing molecule, the atomistic simulation is capable of constructing a complex network structure via crosslinking the LCP monomers.

Figure 3:
Time-dependent simulation to obtain molar fraction of cis-azobenzene at the surface of MD-RM257-10 and MD-RM82-10 thin film samples (thickness: 20 μm) [5]

Figure 4:
(a) Reversible conformational change of the azobenzene and (b) dihedral potential energy functions to simulate the photo-isomerization using MD simulations [6]



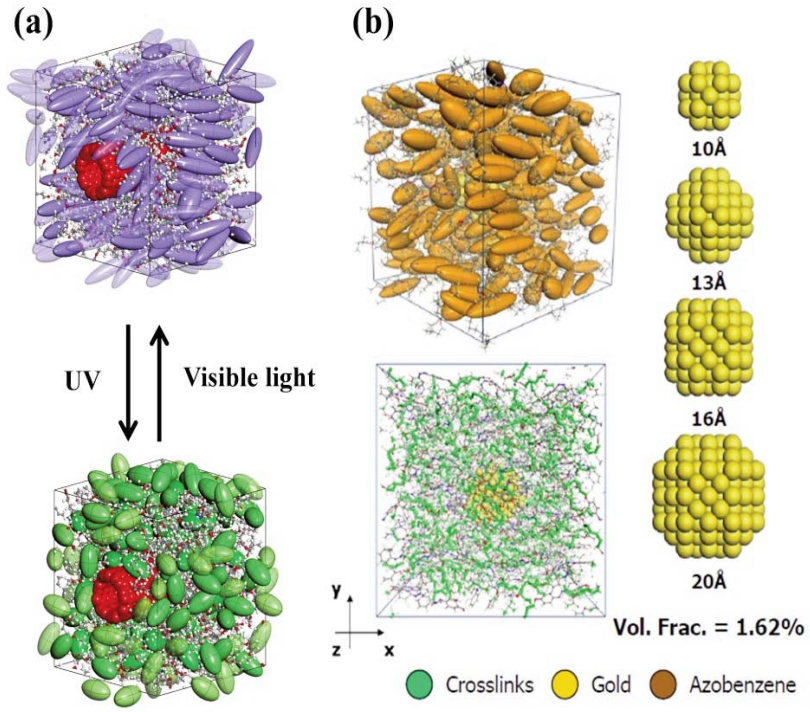
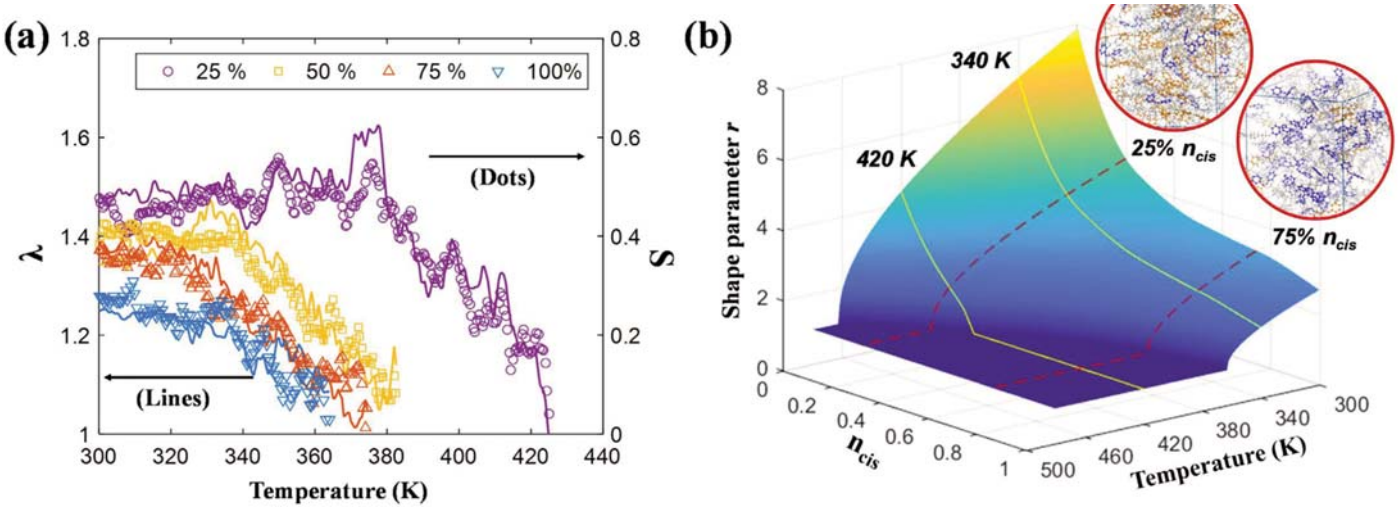


Figure 5:
Azobenzene-containing PRP nanocomposites with (a) carbon nanotubes and (b) gold nanoparticles. [7, 8]

To describe the geometric change of the azo groups induced by the photo-isomerization, we adopted a switchable potential formalism in the MD simulation. As seen in *Figures 4(a)* and *4(b)*, the equilibrium dihedral angle of the azo-dye molecules (C-N=N-C) is switched from 180° to 0° or vice versa [6]. To examine the correlation between the degree of the isomerization and opto-mechanical deformation, we constructed the equilibrated states with a different number of cis-molecules. The presented scheme of the molecular-scale simulation was adopted to examine the reinforcing effect of nano-fillers (gold nanoparticles and carbon nanotubes) on the opto-mechanical behavior of the photo-responsive nanocomposites *(Figure 5)* [7, 8].

The increase in the number of the kinked cis-molecules not only collapses the

Figure 6:
(a) Changes in the shrinkage parameter and nematic order parameter S during the heating-up simulation with different fractions of cis-molecules, and (b) variation of the shape parameter r with respect to the photo-isomerization ratio and temperature [9].



rotational symmetry of the LC molecules by a nematic-to-isotropic phase transition, but also changes the shape of the overall polymer network. This phenomenon was monitored by calculating two key parameters, which are an orientational order parameter (S) and a cell-shrinkage parameter (λ). The orientational order parameter characterizes the long-range symmetry of mesogenic alignment; it ranges from 0 (no directionality) to 1 (perfect alignment). The shrinkage parameter was defined as the fractional change in length of the MD unit cell to the point where the order-clearing temperature T_c^0 is reached. *Figure 6(a)* shows the changes in S and λ induced by both light irradiation and thermal stimuli. It shows a linear relationship between the optical order and polymeric conformation (λ = 1+αS). A nematic-order to polymeric-shape coupling parameter α and thermotropic phase transition temperature were expressed as a function of the photo-isomerization ratio to define the thermo- and opto-mechanical deformations [9]. The shape parameter (r) of the PRP network, which indicates the extent of the shape anisotropy of the LCP molecules, was expressed as a function of the cis-population and temperature *(Figure 6(b))*. These microscopic structural features obtained from the atomistic simulations were transferred to the continuum scale calculations.

A scale-bridging approach was adopted to up-scale the microscopic changes observed via the QM and MD calculations. They were then implemented in the nonlinear FEM to simulate macro-scale photo-bending behavior of the PRP with a specified temperature T and light intensity I_0. The distribution of the light intensity and the associated profile of the cis-concentration with respect to the penetration depth z can be obtained by DFT simulations as stated above. Next, the shape parameter r (equal to λ^3), which was computed using the MD simulation, was embedded into the continuum-scale constitutive equation of the photo-mechanics to describe the variation of the microstate during light irradiation. Finally, the macroscopic bending deformation was computed with geometric nonlinear shell elements [9]. *Figure 7* shows the deformation of a cantilevered PRP strip with different external conditions. The results indicate that the light-induced deformation is significantly affected by varying the stimuli. Furthermore, the proposed multi-scale framework can be applied to simulate the light-induced deformation of PRP with imprinted nematic defects. As seen in *Figure 8* [10], the resulting topographies were found to agree well with the experimentally reported [11].

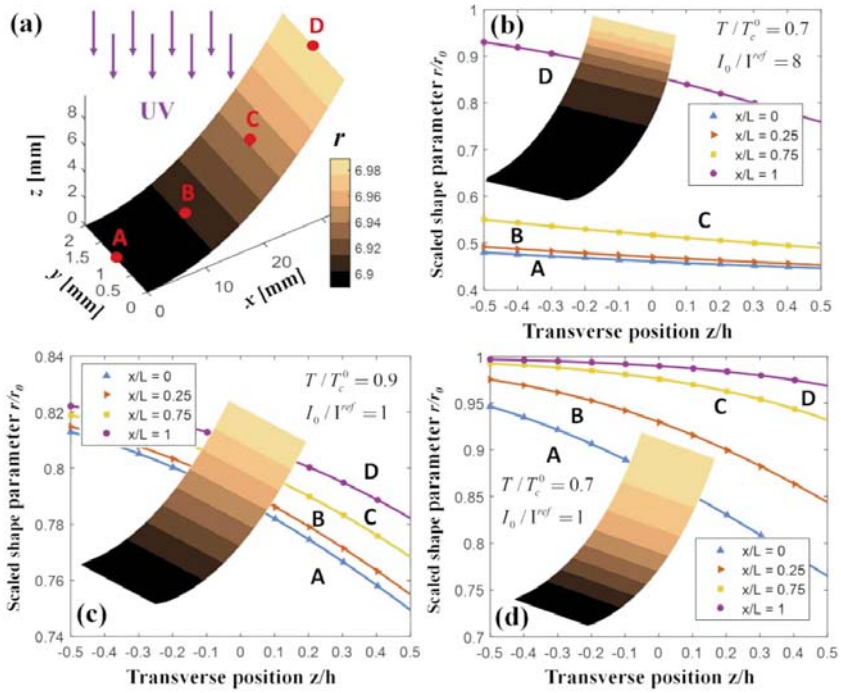


Figure 7:
Photo-bending of the PRP network with different temperatures and light intensities. For equally spaced positions (A-D), the normalized shape parameter is plotted against the transverse position. The light is traveling in the –z direction, h represents the thickness of the film [9]

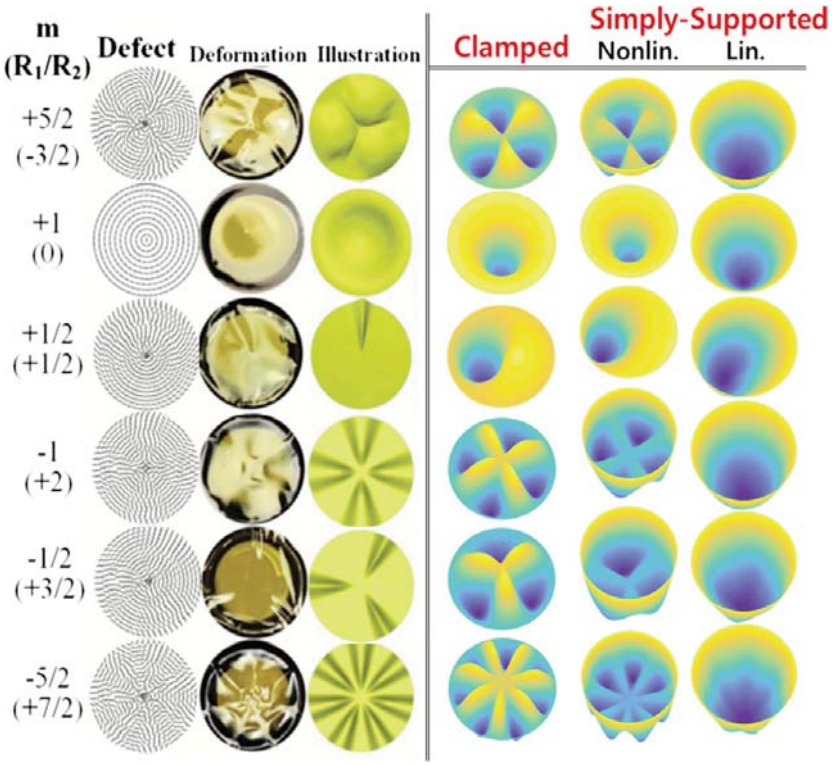


Figure 8:
Light-induced textures of the PRP with given disclination [10]. Experimental surface topography [11] was well reproduced by the multi-scale FEM computations

" analysis and design of the light-induced deformation of the PRP with the aid of the multi-scale computational framework."

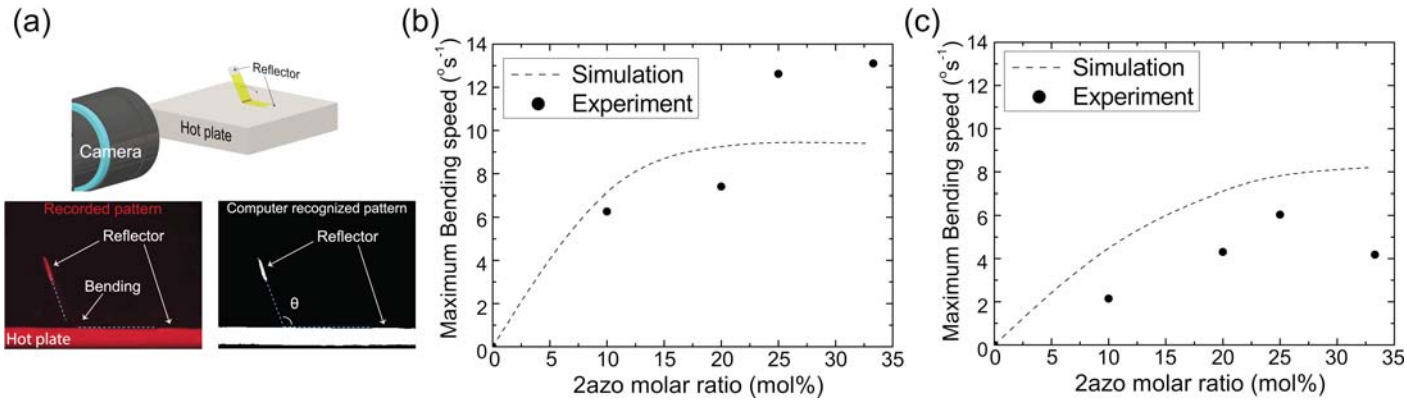


Figure 9:
(a) Schematic of the PRP used for pattern identification, and measuring bending speeds. Simulated bending speed (dash line) compared with experimental observations (black circles) for (b) RM 82 and (c) RM 257 azo-PRPs [5]

The results of the multi-scale simulations were directly compared with experimental results [5]. As shown in *Figure 9(a)*, the photomechanical performance of the azobenzene-incorporated liquid crystalline polymers was captured and identified using the MATLAB image-processing toolkit. Time evolution of the photo-isomerization ratio obtained using the QM calculation was incorporated into the Euler-Bernoulli beam equation to predict the photo-bending speeds of the film. The obtained maximum bending speeds of the responsive polymer are summarized in *Figure 9(b)* and *9(c)* with the simulation predictions. As shown, not only did the simulation successfully predict trends as the composition changes in the polymer, but it also provided quantitative prediction of the 2nd-order velocity values. Eventually, this high-accuracy simulation technique assisted us in effectively programing the smart polymer through partial light irradiation.

" simulated photo-bending behavior of the PRP with various external conditions agreed well with experimental results, thereby demonstrating the high accuracy of the developed scale-bridging method"

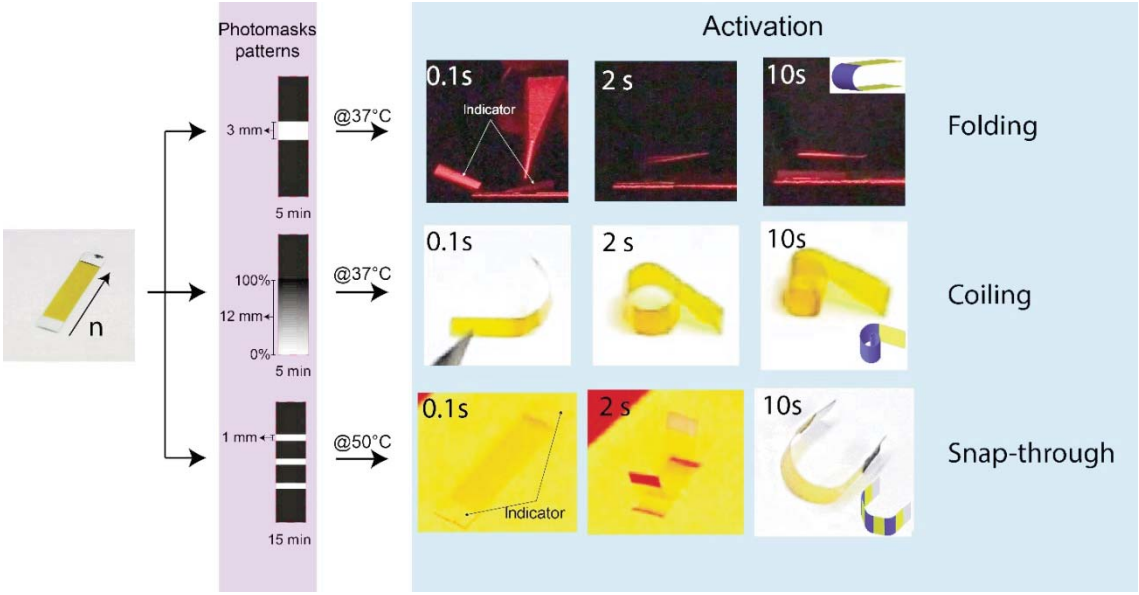
The user-defined deformations were encoded by attaching patterned masking layers to the PRP film *(Figure 10)*. As shown, various 3D complex deformations (folding, coiling, and snap-through) could be implemented within one sample using the photo-masks created with computer-assisted design

In summary, we presented analysis and design of the light-induced deformation of the PRP with the aid of the multi-scale computational framework. The micro-scale response of the photochromic molecules and corresponding shape change of the polymeric network were observed using the quantum- and molecular-scale simulations. Those were systematically incorporated into the finite element analysis to predict the macro-scale deformations. The simulated photo-bending behavior of the PRP with various external conditions agreed well with experimental results, thereby demonstrating the high accuracy of the developed scale-bridging method. The proposed multi-scale simulation technique can be used to effectively design the soft photo-deformable structures.

Acknowledgements

This work was supported by a grant from the National Research Foundation of Korea (NRF) funded by the Korea government (MSIP) (No. 2012R1A3A2048841). ●

Figure 10:
Folding, coiling, and snap-through bending deformations realized by computation-assisted photo-encoding on the same PRP materials



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Advanced Finite Element Techniques for Multiphysics and Multiscale Simulations

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Numerical simulations have been extensively explored during the last half-century and they are now generally accepted as essential tool in the understanding of physical phenomena. Furthermore, motivated by the persistent growth of computational capacity and greater aspirations in Science and Engineering, new challenges requiring innovative techniques are persistently appearing. In this direction, the purpose of this article is to give an overview of recent advanced tools incorporated in a FE code, named as NeoPZ, for the combination of different approximation spaces in a same simulation, by a systematic and generic manner, for multiphysics applications, and tools for multiscale simulations, allowing the coupling of multidimensional phenomena, and complex meshes, combining different element geometries, refinement patterns and polynomial degree distribution.

NeoPZ is a general FE approximation software, in continuous evolution, which has been under development for more than 20 years [5]. It is developed in the object-oriented programming language C++, and is an open-source project incorporating a variety of element geometries (in one, two and three dimensions), variational formulations, and approximation spaces. It implements arbitrary high order approximations [6], and allows the user to apply hp-strategies, without limitations on hanging sides and distribution of approximation orders [2], curved and surface elements [4, 7]. Independent modules offering the basic necessary functionalities of a FE code form it. Namely:

1. Construction of a FE mesh formed by the geometric elements and approximation spaces.
2. Use the approximation spaces to implement a discretized version of the variational statement of the problem in terms of an algebraic system of equations.
3. Resolution of the algebraic system of equations.
4. Post-processing.

NeoPZ is also integrated with pthreads and thread building blocks for efficient execution on multi-core computers. A schematic representation of the independent class modules of NeoPZ is shown in *Figure 1* and is summarized in the next sections.

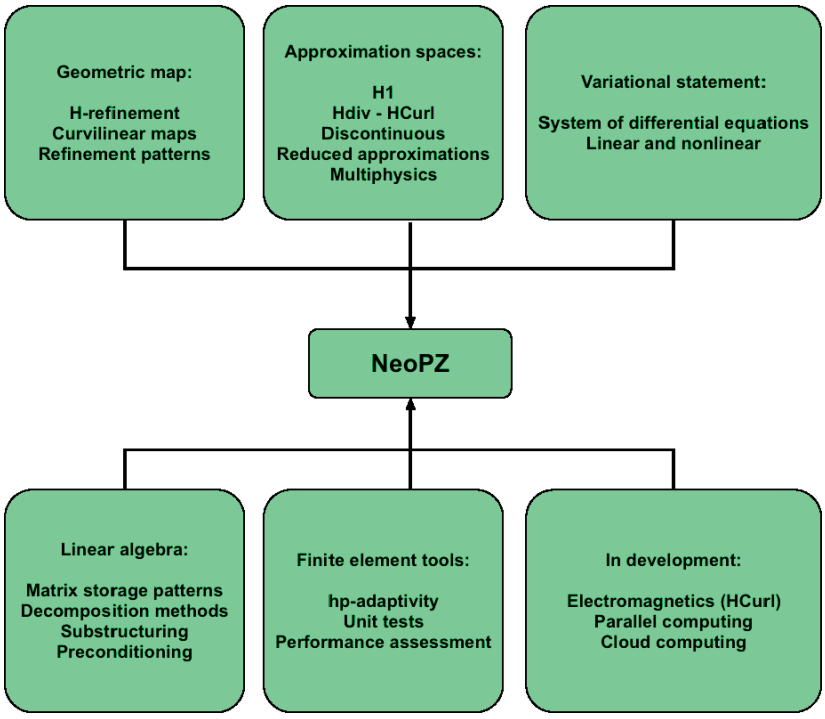


Figure 1: *Schematic representation of class modules of NeoPZ involved in the main stages of the FE method*

NeoPZ structure: main aspects

One of the main characteristics of NeoPZ is its strong separation between geometric map, approximation space, and variational statement. An essential ingredient of finite element simulations is the partition of the computational domain in elements that can be mapped from one of the standard topologies (i.e. master element space). In the NeoPZ environment the elements are represented by triplets of topology-geometry-shape classes associated with point, linear, triangular, quadrilateral, hexahedral, prism, tetrahedral and pyramid spaces.

Topology - The topology class associated with an element defines the master element space and parameter transformations between the parameter of

a point on a side and the parameter of this same point in the volume of the element. The topology class is also responsible for creating an integration rule capable of integrating a polynomial of a given degree.

Geometry - The geometry class is derived from the topology class and has as additional attribute to compute X and ∇X as a function of a parametric point. Many geometry classes can be derived from a single topology class: for instance a *TPZGeoLinear, TPZQuadraticLine, TPZArc3D*, and *TPZEllipse3D* are derived from *TPZLine*.

Shape - The shape class, derived from a topology, implements a method for computing shape functions associated with the topology at a given point. The values of the shape functions depend on the identifiers of the corner nodes, and the polynomial order associated with each side.

Geometry class should not confound with the geometric element class. The geometry class is not aware of the mesh, or its neighbors. Its only attribute of value is to compute X and ∇X. One valuable geometric map is the blend geometric map. It is a nonlinear map where the map of one or more sides is determined by the neighboring element. For instance if a one dimensional arc map is neighbor of a quadrilateral blend element, then the blend geometric map will extend the arc shape of the one dimensional element into the interior of the quadrilateral element. The same holds if this arc element is neighbor of a hexahedral element. In this case the circular arc will extend in the volumetric element.

Geometric element. The computation of the map between the master element and deformed element is delegated to the geometric element class. The root class is the virtual *TPZGeoEl* class. The specific behavior is implemented by *TPZGeoElement <class TPZGeom>* class. By changing the template class, a host of geometric maps can be defined. New instances of the template class can easily be added to the library. The specific attributes of the *TPZGeoEl* class are:

1. *Neighboring information -* two geometric elements are neighbors along a side if they share the points associated with the side. As many elements may share a given set of points, a geometric element may have any number of neighboring elements along a given side. For instance the set of neighbors along a geometric node is the set of elements/side, which contain the node. The neighboring information is kept in a circular list: each element keeps track of one neighbor along each side. The neigh boring information will be crucial to compose the computational elements and to keep track of the necessity of computing shape function restraints for irregular meshes.
2. *Father and son information -* each geometric element with refinement capability keeps track of father and son indexes.
3. *Refining elements with nonlinear geometry -* when refining an element with nonlinear geometry, the sub elements need to conform to the nonlinear geometric map of the father element. The class *TPZGeoElMapped* defines the map of the sub element as a (bi-) linear map in the master element space of the father element. As such the geometric map of this class is defined in a two step process:

$$\zeta_{son} \rightarrow \zeta_{father} \rightarrow X(\zeta)$$

Approximation space. The key feature of finite element approximation is the definition of an approximation space of finite dimension that is a subspace of an infinite dimensional space. One of the main evolutions of the understanding of finite element approximations is the understanding of the approximation properties of different families of approximation spaces. General purpose finite element libraries should give the user the capability of choosing the approximation space. This is a strong motivation to separate the description of the mesh geometry from the definition of the approximation space. Within the NeoPZ library, the computational mesh is composed of a set of computational elements. The computational elements define an approximation space associated with a geometric element. Unless otherwise stated, the approximation spaces are available for all element topologies and any order of polynomial approximation. Shape function restraints are implemented to allow for hanging nodes. The users can create different kinds of approximation spaces, such as H^1 ([6]), H(div) ([3]), H(curl) or discontinuous approximations. Interface elements compute an integral combining function spaces from the two elements sharing an interface. It is used to compute the interface integrals for discontinuous Galerkin methods or hybrid

" The strong separation of the geometric map from the definition of the approximation space and variational statement allows the library to be applied to the numerical approximation of virtually any system of partial differential equations."

approximations. There are also special purpose approximation spaces. For instance, reduced approximation uses spaces created as a linear combination of a set of approximations generated by a conventional setting. It has been successfully applied to hydraulic fracturing simulations [10] and to model geomechanics coupling [8] in flow through porous media. These approximation spaces are suited for the solution of specific problems and yield very accurate solutions at reduced computational cost.

Variational statement. Finite element approximations can be viewed as Galerkin approximations of weak statements applied to conservation laws where the subspace is generated in a way that has been described above. The weak statement that needs to be approximated depends on the physical phenomenon one wants to approximate, its variations are innumerable. The transformation of the weak statement into an algebraic system of equations is obtained by the assembly of element contributions. The element matrices are computed as an integral over the domain of the master element. The integral is computed numerically and, as such, each element matrix is obtained as the sum of contributions at integration points. The contributions depend essentially on the weak statement that is being approximated. *TPZMaterial* class is the root class of the classes that compute the contribution (at an integration) point of a weak statement as a function of the set of shape functions and their derivatives. Its main methods are:

1. *Contribute* - computes the contributions to the tangent matrix and right hand side at an integration point.
2. *ContributeBC* - computes the contributions to the tangent matrix and right hand side of boundary conditions.
3. *ContributeInterface* - computes the tangent matrix and right hand side of a discontinuous Galerkin weak statement associated with the interface between two elements. *TPZMaterial* class also includes interfaces to compute post-processed quantities of interest.

Linear Algebra. Finite element computations are essentially composed of a sequence of matrix operations. Object oriented language facilitates the management of data structures, but the bulk of operations are matrix related. In the view of the NeoPZ library, the only mandatory a matrix object needs to implement is a linear transformation. At the root of derivation tree is the *TPZMatrix* class that defines the computational interfaces, the derived classes may or may not implement. *TPZFMatrix* class represents a full matrix and is a storage declared object (column maior). A large number of classes representing different matrix storage patterns are derived from TPZMatrix class. Depending on the library linked with the environment

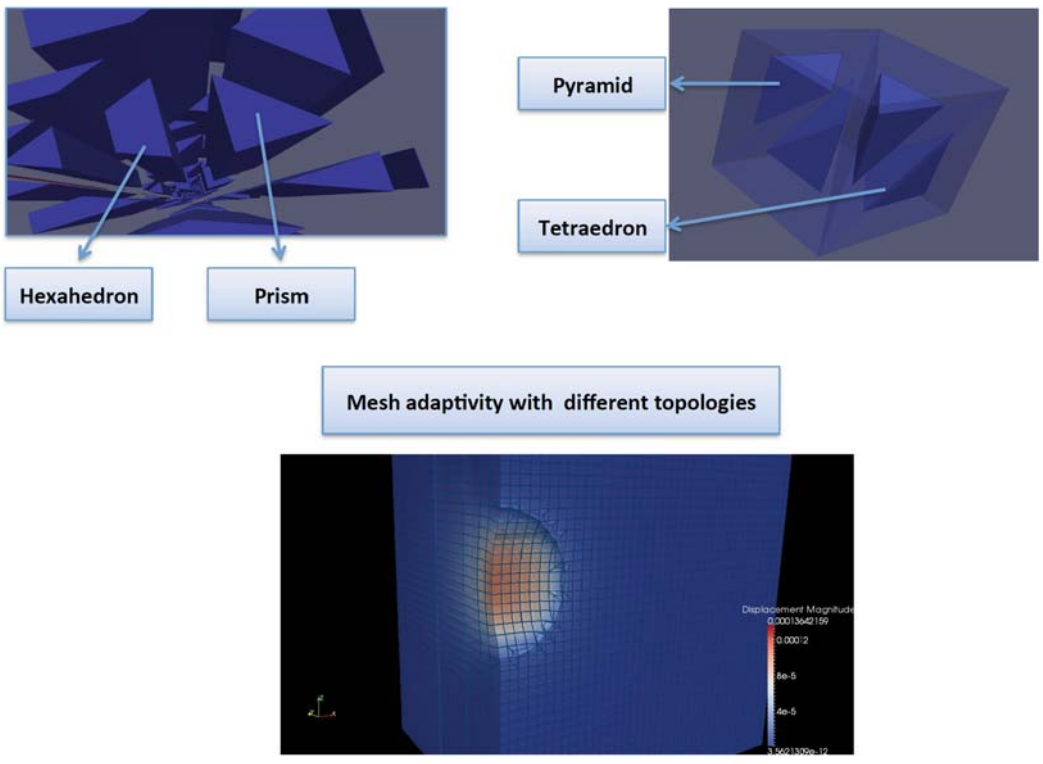


Figure 2: *Directionally refined mesh towards a fracture contour, combining different element geometry*

(i.e. Lapack, Blas, MKL), multiplications, decompositions, etc., access the highly efficient implementations of these libraries. The matrix classes are strictly separated from the finite element computations. No class derived from *TPZMatrix* is aware of the finite element classes. A separate derivation tree makes the bridge between the matrix classes and finite element computations. *TPZStructMatrix* is the root class for all classes that can build a global matrix from a mesh object. *TPZFStructMatrix* builds a full matrix by assembling the element stiffness matrices. *TPZBndStructMatrix* builds a band matrix, *TPZSpStructMatrix* builds a sparse matrix, and so on.

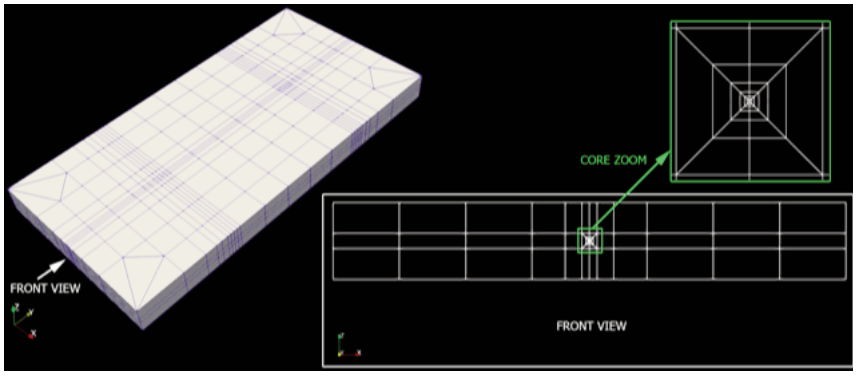


Figure 3:
Directionally refined mesh around a horizontal well in a rectangular drainage area

NeoPZ advanced techniques

Recently, new advanced techniques have been incorporated into NeoPZ, allowing the simulation of more complex phenomena. Some of them are briefly described here.

Combined geometry and directional refinement patterns. The division of an element into a fixed number of sub elements can lead to suboptimal refined meshes. In many problems the solution shows sharp gradients in a single space direction, as is the case of solutions with boundary layers. The h-refinement capability of the object-oriented library has been extended by the introduction of refinement patterns. A refinement pattern is a mesh whose first element is a master element and the remainder of the mesh is a partition of the first element. This mesh defines the refinement that is going to be applied to the element. This extension gives the user total freedom on how elements can be divided. Tools have been added to ensure that neighboring elements are refined in compatible patterns. When directional refinement patterns are applied, the sub elements have different types of element topology, as illustrated in *Figure 2*, corresponding to an application of hydraulic fracture propagation, where a directional refinement pattern is used to improve the representation of the fracture front [10]. *Figure 3* refers to a mesh used for the simulation of a porous medium limited by a rectangular drainage area. The oil pressure is characterized by a strong decay from lateral boundary towards the well, motivating a directional refinement.

Multiphysics elements Many relevant physical phenomena need to model the interaction of different conservation laws to yield meaningful results. The challenge is to apply specific families of approximation spaces may better model different conservation laws. This kind of approximation space combination can now be coherently integrated in NeoPZ, in a systematic and generic manner [9]. For instance, the implementations of the mixed formulation of Poisson problems, presented in the recent papers [4, 3, 7], have been facilitated by this new capability.

For the coupling of geomechanics and multiphase fluid flows in porous media, the combination of continuous approximations (for solid deformation), discontinuous approximations (for components transport or fluid pressure) and H(div) (for Darcy's flux) were used, as illustrated in *Figure 4*. Several multiphysics applications in reservoir simulations have been developed in [8]. In [10] a hydraulic fracture is approximated by considering the interaction of a 3D elastic structure with the fluid flow inside the planar fracture.

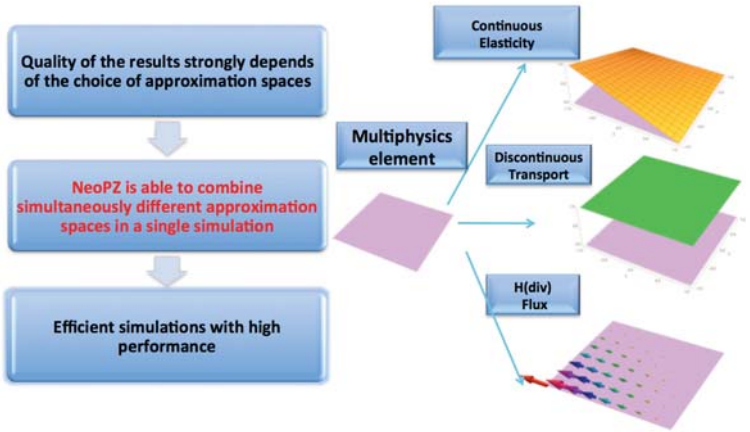


Figure 4:
Multiphysics element for fluid flow in porous media coupled with geomechanics

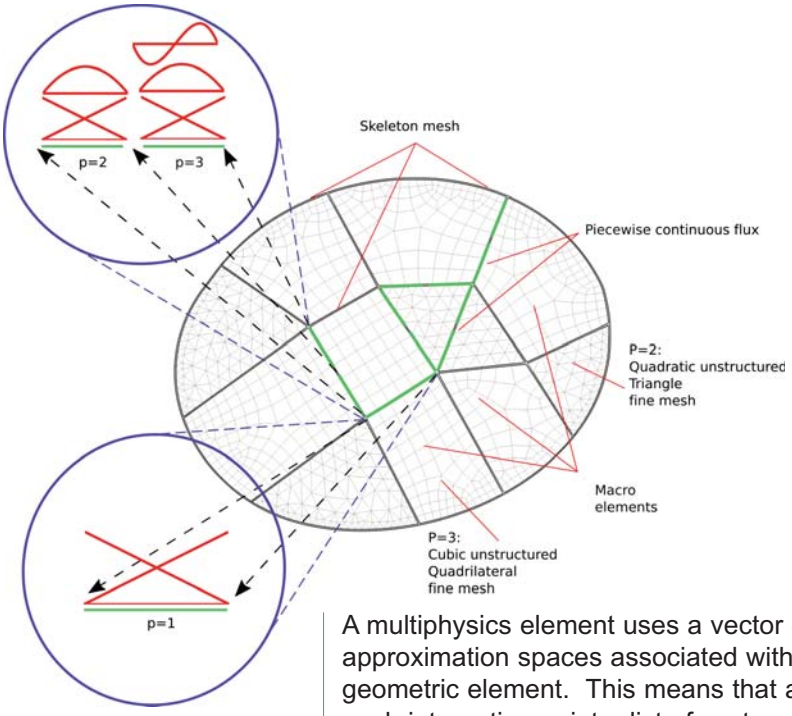


Figure 5: *Diagram illustration of MHM meshes*

A multiphysics element uses a vector of approximation spaces associated with a geometric element. This means that at each integration point a list of vectors of shape functions and derivatives are computed. This set of approximation space is used by the *Contribute* method of the *TPZMaterial* class to implement the variational statement.

Multiscale Hybrid Mixed (MHM) simulations MHM approximations are obtained by relaxing the a priori continuity constraint, by including a Lagrange multiplier, defined on a macro skeleton mesh to weakly impose the solution continuity. In a MHM context [1], the state variables are defined at different scale levels. The sketch in *Figure 5* illustrates the kind of complex mesh structure is used in MHM simulations. NeoPZ can be used to implement this type of formulation. MHM requires the combination of approximation spaces associated with different domains, refinements, and heterogeneous polynomial degree distributions.

Elements of varying topology are used in each domains. Elements at different geometric refinement can be used as long as the original root mesh is unique.

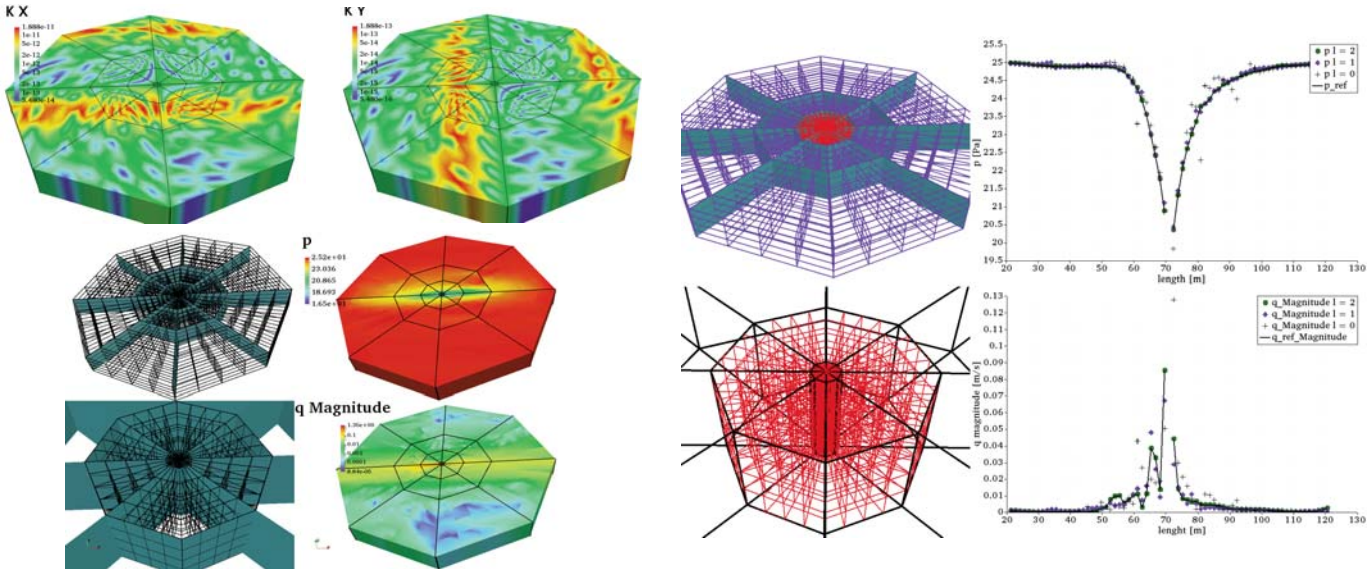
In its original formulation [1], the MHM method was designed with H^1 –conforming approximations to resolve the fine structures inside the macro-elements (down-scaling stage). Another variant MHM-H(div), which is locally conservative at any scale, was developed for reservoir simulations with rock heterogeneities, showing very efficient results in [8].
Like several fine-coarse approaches, the method incorporates the effects of fine scales to calculate velocity and pressure in a coarse resolution, to later calculate detailed velocity fields.

This technique has been used to represent the flow in a radial reservoir with a highly oscillatory permeability field, as shown in *Figure 6*. The graphs comparing a reference fine mesh approximation and MHM-H(div) approximations for pressure and velocity at macro scale levels l, computed over a diagonal line. MHM-H(div) method has been applied to the approximation of a pressure field on a rectangular section of an oil reservoir, with one injector and one producer oil wells. After static condensation, the 3D problem was simulated with 16,994 degrees-of-freedom, contrasting with 2,649,776 total degrees-of-freedom of the MHM-H(div) model. This result demonstrates the computational efficiency of the MHM-H(div) method.

Conclusion

In this article we described the essential features of the NeoPZ library, which have contributed to making it a general purpose finite element library. The strong

Figure 6: *MHM-H(div) application: high oscillatory permeability field, approximated pressure and flux variables, MHM meshes, and comparison error plots*



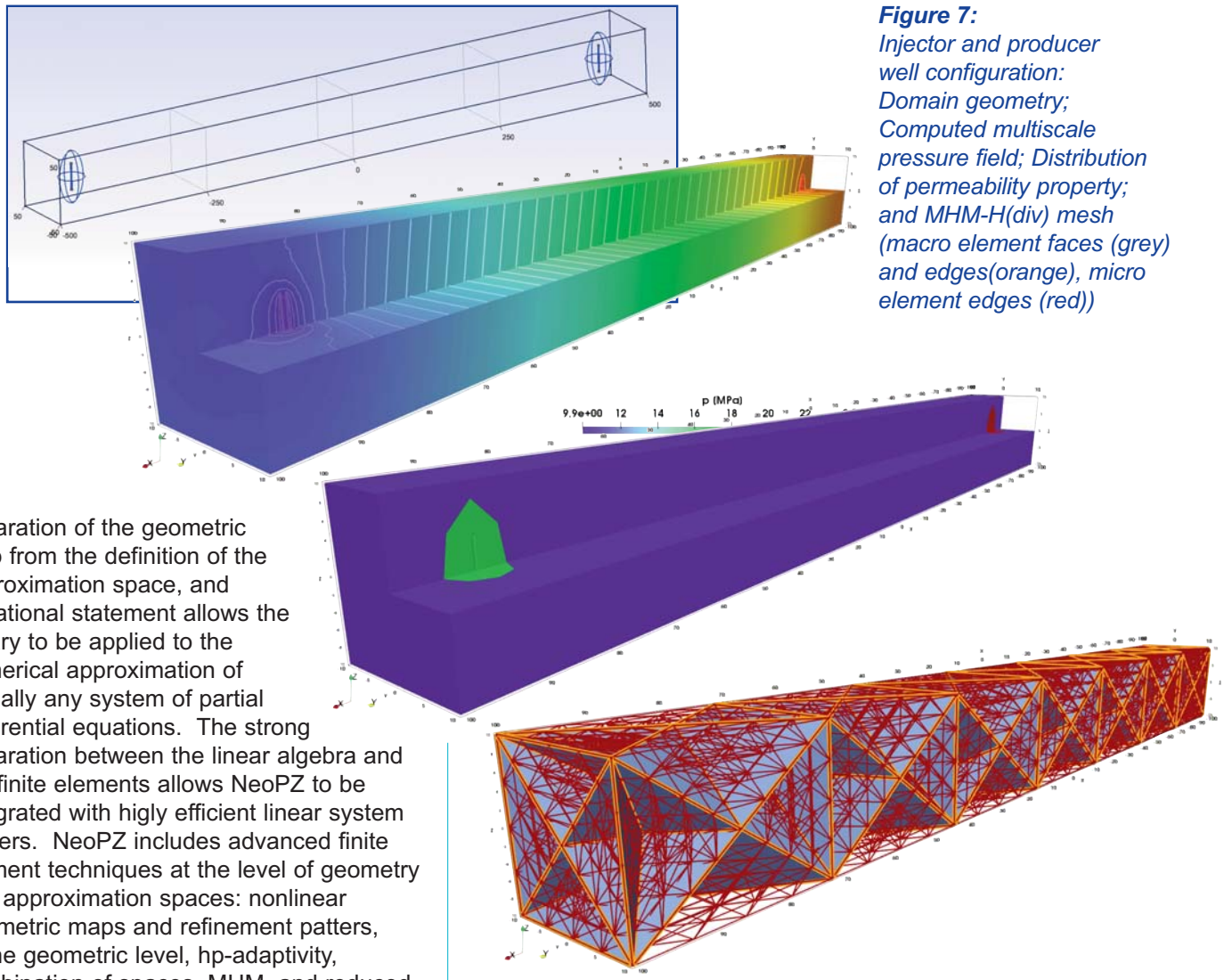


Figure 7:
Injector and producer well configuration: Domain geometry; Computed multiscale pressure field; Distribution of permeability property; and MHM-H(div) mesh (macro element faces (grey) and edges(orange), micro element edges (red))

separation of the geometric map from the definition of the approximation space, and variational statement allows the library to be applied to the numerical approximation of virtually any system of partial differential equations. The strong separation between the linear algebra and the finite elements allows NeoPZ to be integrated with higly efficient linear system solvers. NeoPZ includes advanced finite element techniques at the level of geometry and approximation spaces: nonlinear geometric maps and refinement patters, at the geometric level, hp-adaptivity, combination of spaces, MHM, and reduced spaces at the approximation space level.

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Computational Hemodynamics at Extreme Anatomical Scales

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Introduction and Overview

The development of one-dimensional models dates back to the 50's, where the scientific community became increasingly interested in simulation-based techniques to study physiology while accounting for the multiple time scales and levels of spatial organization featured by the cardiovascular system (CVS). Nowadays, many applications such as diagnosis, treatment and surgical planning have been enormously benefited from these complementary tools.

The level of sophistication behind the mathematical representations has rapidly grown because of two major aspects: the availability of data (mainly in the context of patient-specific simulations) and the availability of massive computational resources. Thus, different approaches have gained momentum according to the level of description required by the underlying question, ranging from 0D (ordinary differential equations) to 3D (three-dimensional partial differential equations). In this context, notwithstanding the ubiquitous availability of high performance facilities and the consensual understanding about the relation between the three-dimensional intricacy of the blood flow and several cardiovascular diseases, even these days are witness of a prolific resurgence of one-dimensional (1D) modeling to simulate systemic interactions which determine pressure and flow rate waveforms, providing an accurate description of the behavior of the CVS at a reasonable cost.

The branching pattern of the CVS and the differential blood flow supply to specific and distributed organs is responsible for the reflections pattern. Such complex architectural assembly of deformable pipes, combined with the pressure loss along the network, shapes the pressure contour from the aortic root to the peripheral vessels. The description of this pressure pulse conformation has been given by many good models proposed in the literature, which have been able to capture the basic features of the mechanisms. However, the need to push the boundaries of CVS research further posed challenges concerning the topological organization of the CVS, aiming at creating more realistic anatomical and physiological descriptions. These challenges amount to conceive a representative model of the CVS to serve as geometric substrate on top of which a physical model can be set up. Clearly, this is a patient-specific problem, given the large inter-individual variability of anatomy and physiology. However, a virtual representative human being is still conceivable based on well-grounded anatomical data. Moreover, such representative virtual human would not only be useful to perform hemodynamics research in the CVS, but also to set the grounds for truly interdisciplinary research capable of integrating biological and mechanical principles. In a nutshell, when a more accurate analysis of the systemic interactions and its implications in cell function and ultimately disease onset and development is sought, a higher definition in the vascular anatomy is required.

Importantly, the definition of a blood flow model of the CVS implies truncating the arterial network at a certain level. Naturally, this truncation introduces limitations to the model regarding the pressure and flow at specific locations in the network, because of the proximity of boundary conditions which can exaggeratedly constrain the blood circulation.

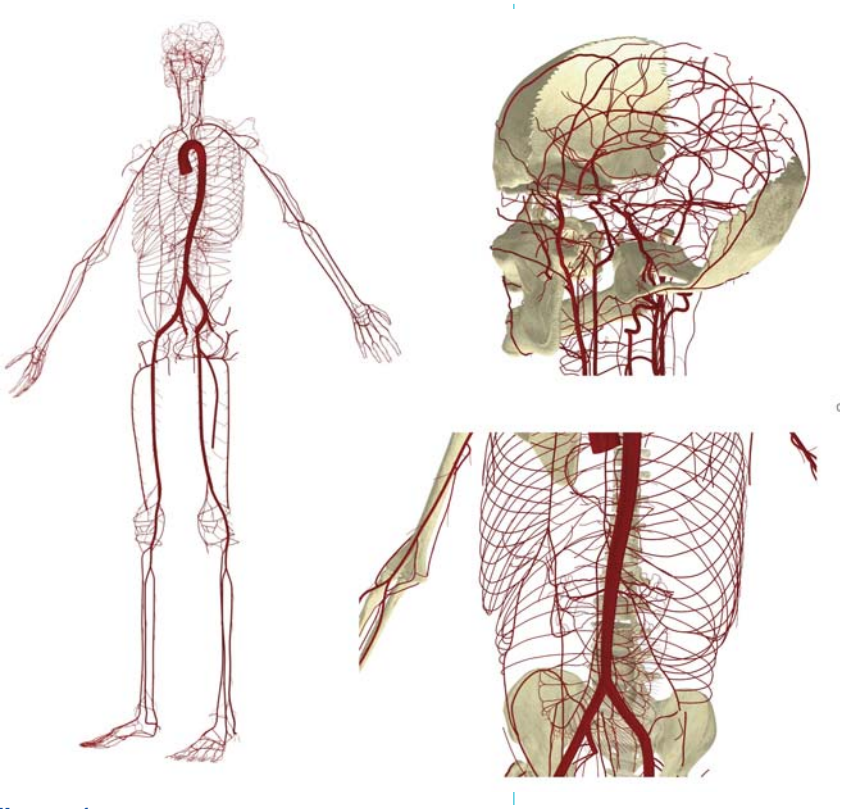
In the context of the previous paragraphs, in the HeMoLab research group (http://hemolab.lncc.br/), we have developed a model of the arterial system called Anatomically Detailed Arterial Network (ADAN) model. This model aims to provide an ultimate patient-generic description of the arterial vasculature by making use of available anatomical data. Using such topological arterial description allows us to assemble a mathematical model for the blood flow whose calibration relies on physiological concepts and published data. In this way, we have been able to create an unprecedented and

groundbreaking computational model of the entire arterial network to set the groundwork to perform cutting-edge cardiovascular research supported by modeling of physical phenomena and simulation-based techniques. The arterial circuitry of the ADAN model has been outlined in the three-dimensional (3D) space in order to deliver an anatomically realistic environment. The model is in compliance with the field of knowledge of descriptive anatomy [13,14]. Remarkably, the level of detailed attributed to the model enables the connection between the vasculature and the so-called vascular territories.

Anatomically Detailed Arterial Network (ADAN) Model

As said, the ADAN model has been built in 3D space using data extracted from classical anatomical textbooks [13,14], featuring the average vascular anatomy of a male subject. Arteries have been constructed on top of a scaffold consisting of a digital dataset of the human skeleton. The model contains 1598 named arteries, plus 544 smaller vessels called perforator arteries which ultimately deliver blood to peripheral regions. The model represents a subject of 170 cm in height, and with an equivalent body surface area 16.488 cm^2 (measured from the surface of vascular territories). Model morphometry is determined by using the scaffold and the specialized literature, while the vessel radii has been gathered after a gargantuan effort to sweep the specialized literature, thus producing a unique data collection complementing descriptive anatomy textbooks.
Figure 1-left features the ADAN model with a detail of the vascularization in the upper region of the body. The model dataset can be accessed freely at http://hemolab.lncc.br/adan-web/.

Blood delivery to specific organs (brain, kidneys, liver, stomach, etc.) is calibrated to match data reported in the specialized literature [15]. In turn, the distributed the regional blood supply to the vascular territories requires refinement according to the perforator arteries that arrive at each of the territories. This mapping between arterial vessels and vascular territories is reported according to [3], and the size of vascular territories determines the amount of blood to be received. *Figure 1-right* shows the concept of vascular territories.



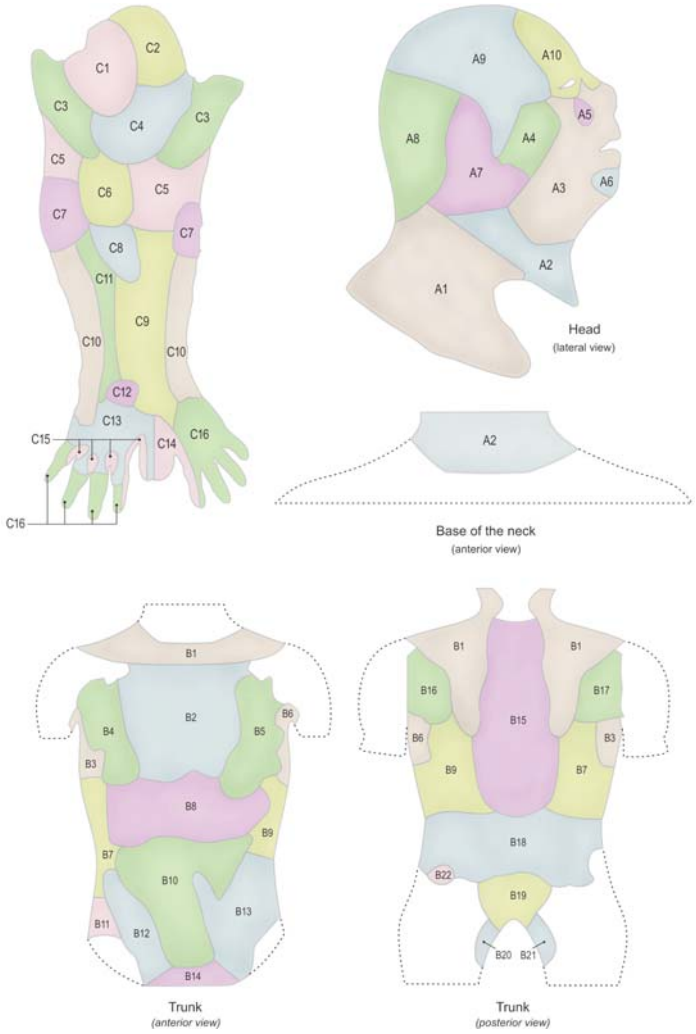
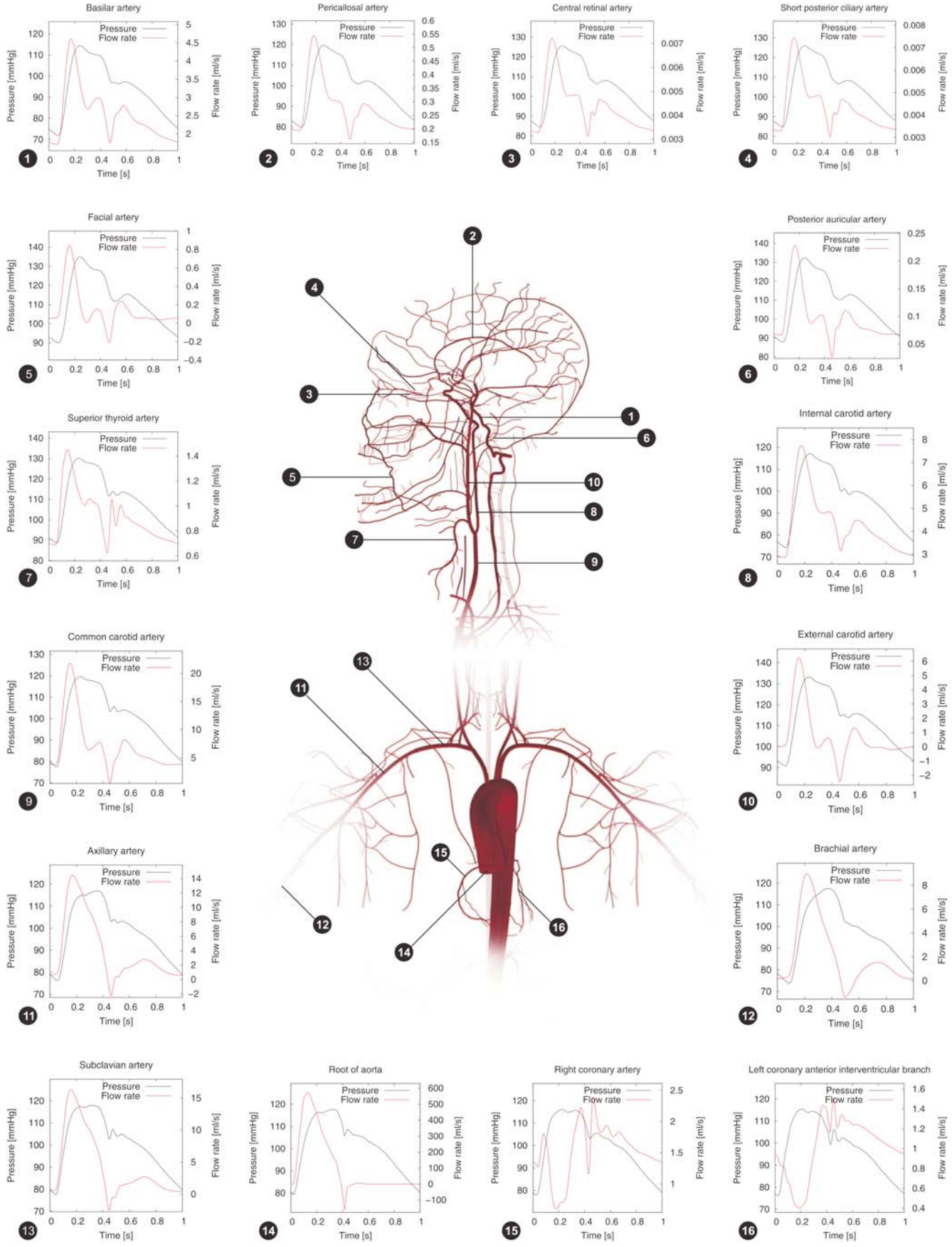


Figure 1:
Above: ADAN model with a detail of the vascular circuits in the brain and abdominal cavity
Below: Concept of vascular territories for the ADAN model

Figure 2: *Hemodynamics predicted by the ADAN model in the upper part of the body*

The mathematical model consists in the classical one-dimensional equations that describe the incompressible flow of a fluid in deformable vessels (mass and momentum conservation laws). Vessels are considered to behave as viscoelastic pipes, where the stiffness is dictated by elastin and collagen contributions. Model parameters are established following the guidelines reported in [4], which rely on specific calibration criteria to define arterial thickness and arterial wall parameters according to the type of vessel under consideration.



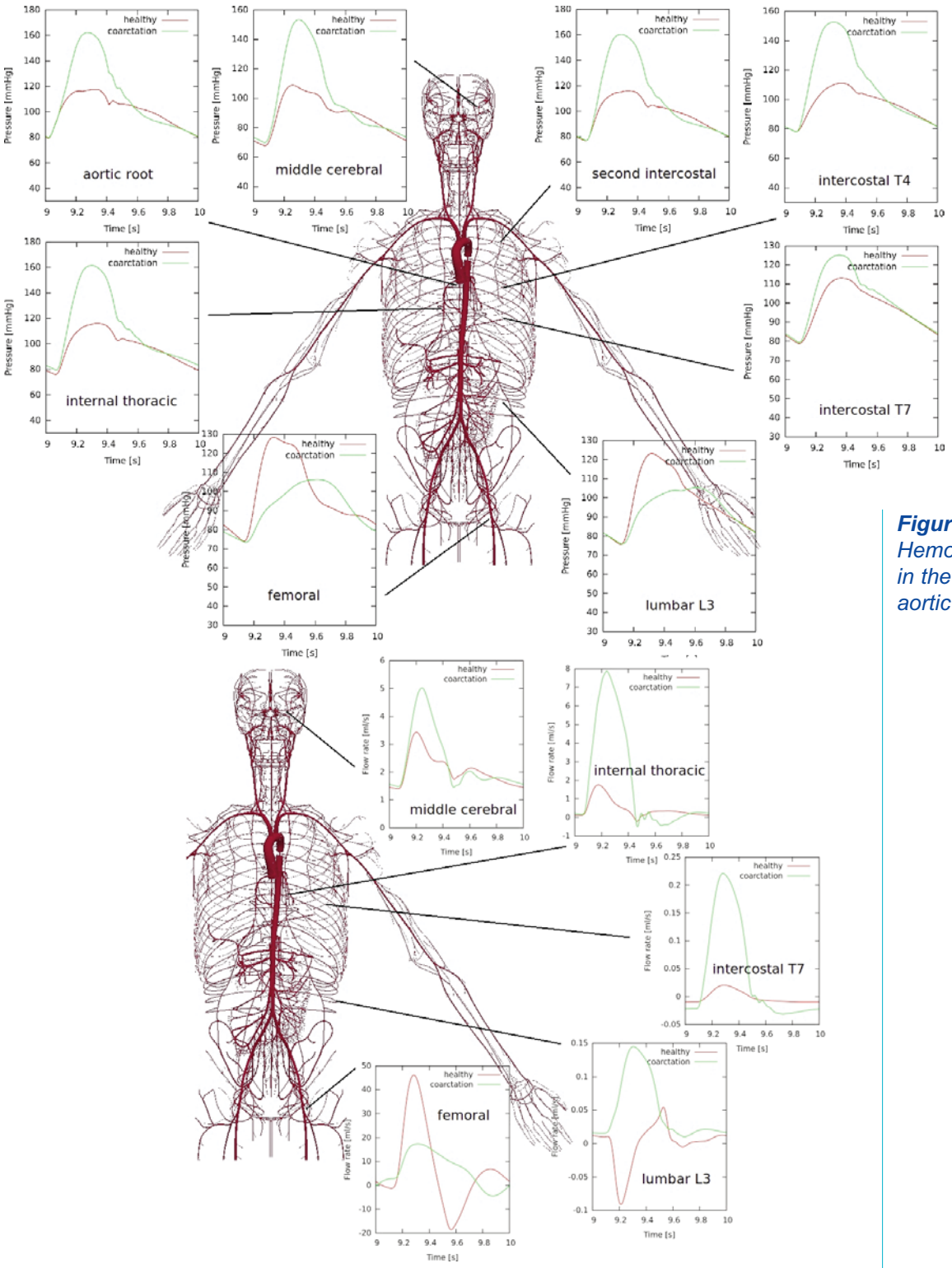


Figure 3: *Hemodynamics in the presence of aortic coarctationt*

Although the model is a one-dimensional model, the numerical solution of the mathematical problem presents substantial difficulties. To overcome this technical difficulty, an explicit finite-volume scheme relying on a Riemann problem solver has been developed. The methodology enables the solution of one-dimensional blood flow models including smooth as well as sharp variations of mechanical and geometrical properties of vessels [9]. In order to solve the problem in a timely manner, a local time-stepping algorithm is employed [10].

Figure 2 gathers the pressure and flow rate signatures for vessels in the head and in the thorax. The study of the variation of these signatures from health to different classes of disease enables to provide mechanistic explanations and the characterization of the model, in terms of variations of model parameters, to cohorts featuring different hemodynamic patterns. This aspect is closely related to the integration of data assimilation strategies fed by clinical data, which turn out to be critical for the success of the patient-specific (or population-specific) utilization of this kind of models [7].

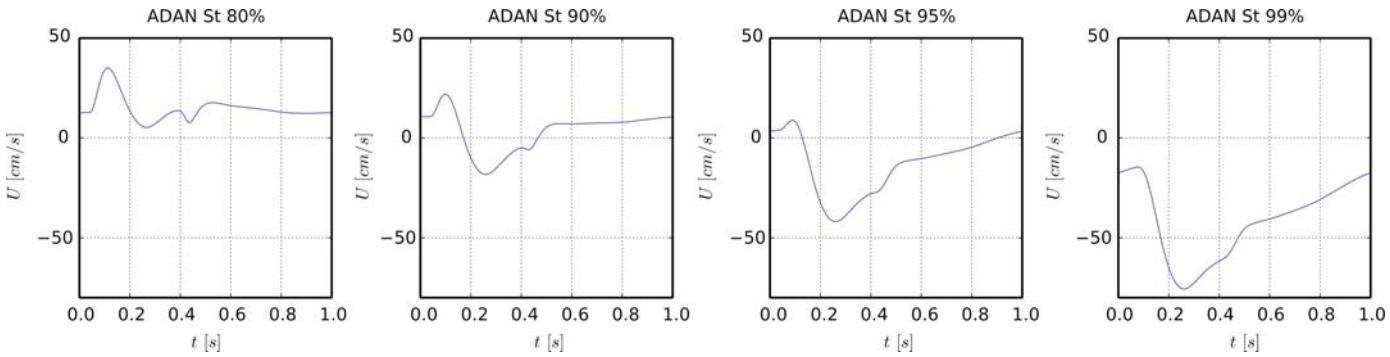


Figure 4: *Modeling of subclavian steal phenomena*

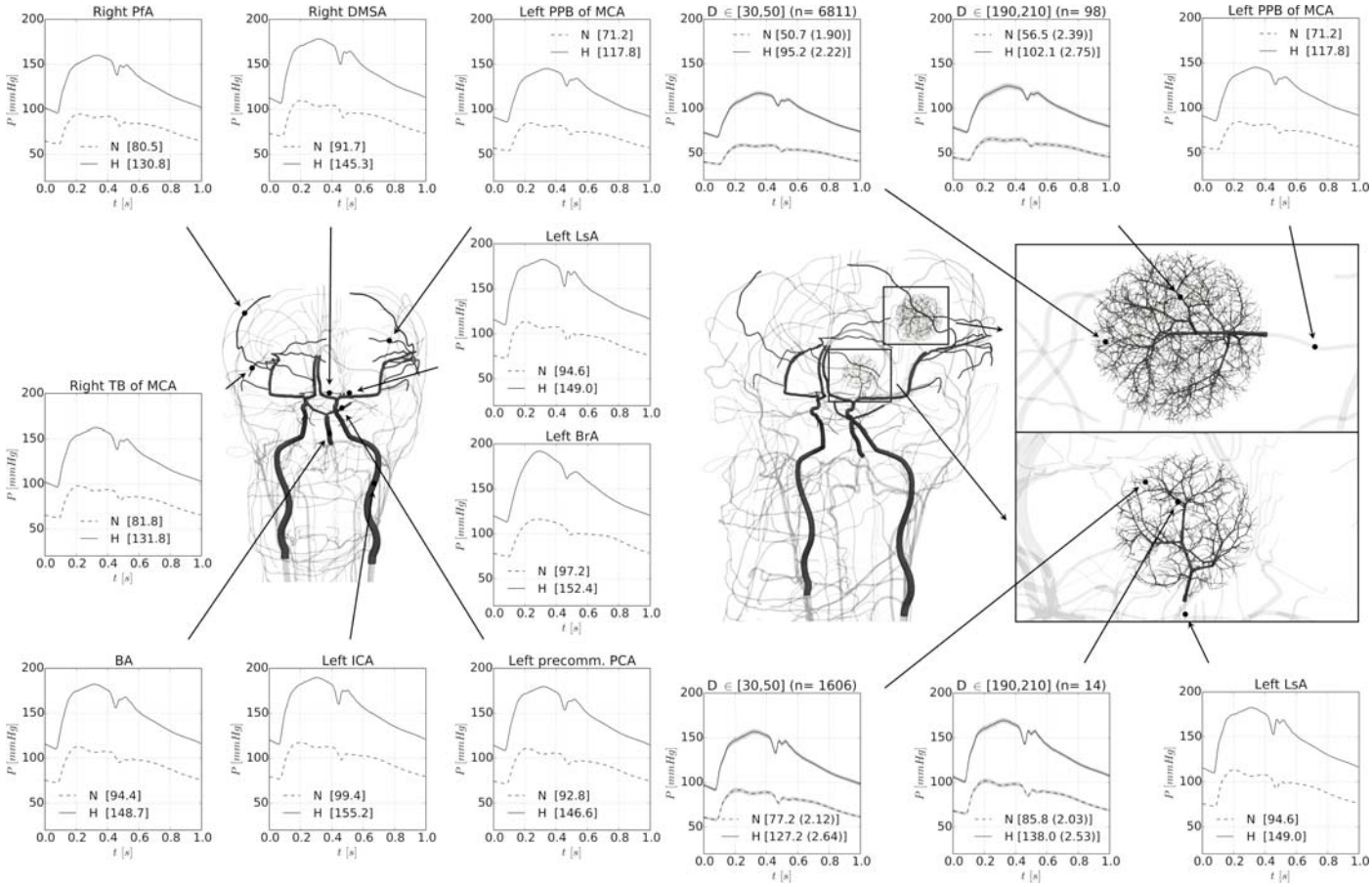
Moreover, the ADAN model is turning into an anatomical and functional atlas on top of which other models can be constructed. This includes the possibility of embed 3D models into the circulatory system to gain insight about the detailed hemodynamics in certain arterial districts as well as the possibility of developing cheaper and easy to handle 1D (or 0D) submodels. Hence, the ADAN model not only provides a virtual laboratory to study the interplay between hemodynamics and vascular mechanics, but also yields a baseline model to verify reduced representations of the cardiovascular system [11,12], as well as to provide benchmarking tools for numerical methods [6].

Computational Hemodynamics

Let us now discuss some applications to illustrate the predictive and descriptive capabilities of the ADAN model.

The first scenario is that generated by the presence of a severe obstruction in the aortic arch, acknowledged as aortic coarctation. This condition produces secondary hypertension, more specifically, high blood pressure in the upper part of the body and reduced blood flow to the lower body. The presence of the intercostal arteries provides a collateral circuit to mitigate the flow impairment to the lower part of the body. Therefore, intercostal arteries grow in diameter even producing rib notching.

Figure 5: *Integration of the ADAN model with CCO networks for simulations arteriolar hemodynamics*



The simulation of such conditions in the ADAN model, by placing a stenosis model at the aortic arch, results in the predictions reported in *Figure 3*, where the healthy and coarctation scenarios are compared in terms of the blood pressure and flow rate waveforms. The upper body hypertensive condition is predicted, as well as the delayed and slow upstroke in the lower body vessels, featuring broad and blunted systolic peak, and no landmark indicating the beginning of the diastole. The appearance of a strong pressure gradient in the intercostal vessels substantially increases the blood flow through these arteries, triggering remodeling and growth processes. These characteristics have been reported in a number of studies performed in animal models.

The second scenario of application consists in the analysis, using the ADAN model, of a condition known as subclavian steal phenomenon. For more information about this problem, the reader is referred to [1]. This condition takes place whenever an obstructive lesion is present in the subclavian artery. This induces a complex compensatory mechanisms in which the flow is diverted through the carotid artery towards the brain and then descends through the basilar and ipsilateral vertebral arteries reaching the distal region of the lesion, and supplying blood to the affected arm. Increasing the blood demand by, e.g., exercising, can lead to small transient neurological symptoms. As shown in *Figure 4*, for varying severities of the subclavian stenosis, the ADAN model is capable of predicting a wide range of waveform flow signatures in the vertebral artery, through which the systolic peak is first reduced, and then becomes inverted (a condition called partial steal), to finally reach a total retrograde flow when the subclavian artery is almost occluded. Model predictions indicate that, in resting conditions, the steal phenomenon develops in the cases of more severe lesions, while the simulation of induced hyperemia in the arm can double the amount of blood stolen from the posterior circulation.

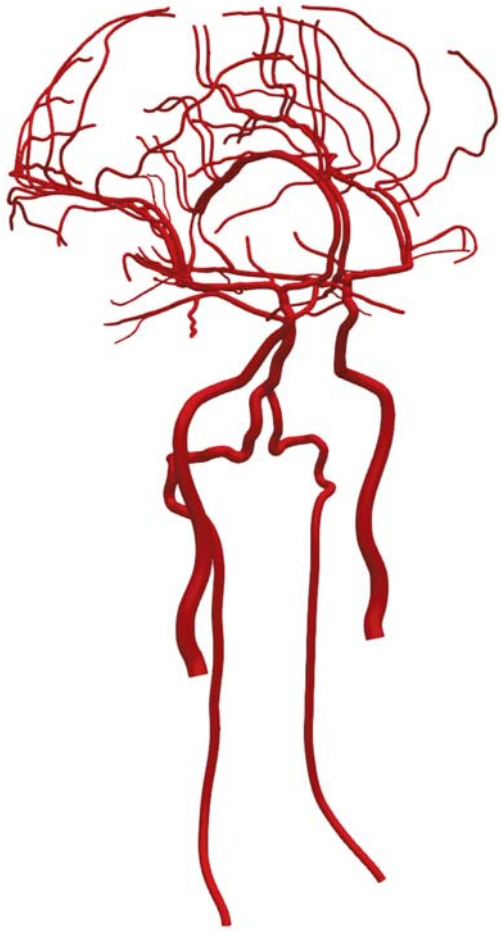
The last scenario consists in the integration of the ADAN model with automatically generated vessels via Constrained Constructive Algorithms (CCO) in order to model the blood pressure in the brain arterioles under hypertensive conditions. For more information about this problem, the reader is referred to [2]. To this end, the vascular mechanics of the ADAN model was altered to represent those conditions. Peripheral networks representing vascular territories in the posterior cortex and at the base of the brain were created and connected to the ADAN model in the posterior parietal branch of the middle cerebral artery and in the lenticulostriate artery, respectively. This kind of study allowed us to describe the pressure gradients in the peripheral beds around the brain, and explain that even under hypertensive conditions, the small vessels over the cortex remain protected from high blood pressure by the pressure drop occurring between the Circle of Willis and the vascular territories, in contrast to lenticulostriate vessels, which are completely expose to high pressure. From this, it would be possible to provide evidences to elucidate specific pathophysiological mechanisms of cerebral small vessel disease in the different regions of the brain. *Figure 5* displays the blood pressure in normotensive and hypertensive conditions for several intracranial vessels and also for the arterioles corresponding to the peripheral territories. The pressure substantially drops from the base of the brain towards the convexity, thus protecting the cortical vessels from being exposed to high pressure.

As a final example we exploit a portion of the 1D arterial skeleton of the ADAN model to construct a 3D model of the brain vasculature. In this case, instead of using traditional 3D discretization techniques we employ a recently developed numerical approach for simulating fluid flow in tubular domains. This method, coined Transversally Enriched Pipe Element Method (TEPEM) [5,8], discretizes the domain into pipe elements with low order axial approximation and high order transversal approximation, and proved to be extremely efficient towards retrieving the main blood flow features. *Figure 6* illustrates the solution (velocity profiles, pressure field and wall shear stress) achieved with the TEPEM. The application to patient-specific geometries is also feasible [8], as well as the coupling of this more detailed with the full 1D arterial system.

Final remarks

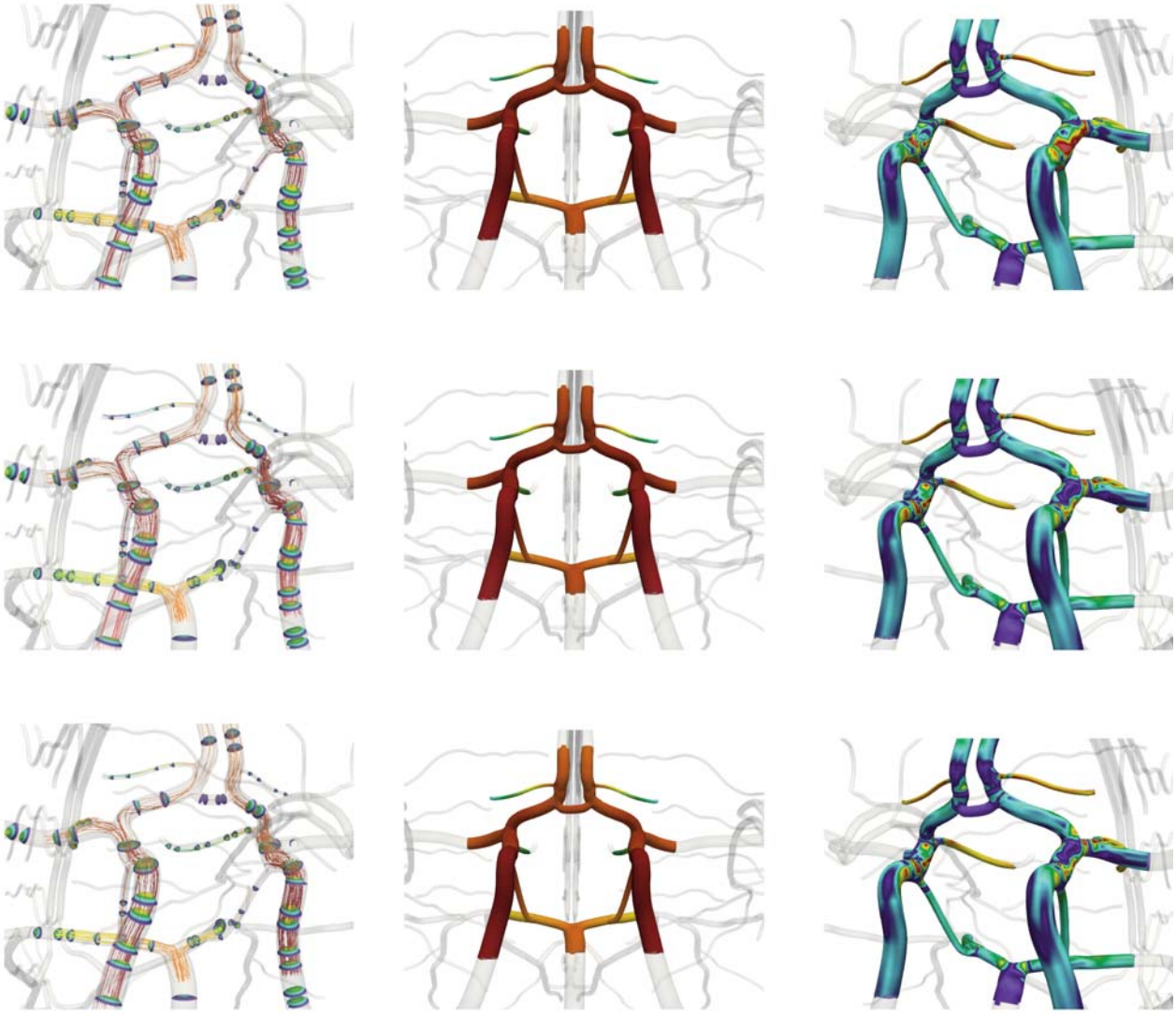
Throughout the last years, we have developed a novel model of the arterial system featuring a high level of anatomical

“ the ADAN model not only provides a virtual laboratory to study the interplay between hemodynamics and vascular mechanics, but also yields a baseline model to verify reduced representations of the cardiovascular system as well as to provide benchmarking tools for numerical methods.”



and functional detail, whose predictions, consisting of pressure and flow rate contours, were verified with the specialized literature. This also triggered a series of contributions in the field of numerical methods to face such scientific computing challenges. In this article we have shown that the ADAN model provides a comprehensive virtual laboratory which can potentially be tailored to model specific cardiovascular conditions. The capabilities have been illustrated here with the application to three pathological scenarios of clinical interest. In the stages to come, the integration of the ADAN model with data assimilation procedures provides a door for the translation into the clinic addressing patient-specific

Figure 6:
Geometry of cerebral arteries from ADAN and blood flow simulation using TEPEM. From left to right:
Velocity profiles and streamlines, pressure and wall shear stress in the Circle of Willis.



cardiovascular modeling. The remarkable feature of the ADAN model is the extremely detailed anatomical description of the arterial network, which enables to tackle, in silico, complex hemodynamic phenomena that remain poorly understood. The natural (vascular) connection provided between the large arteries and the peripheral vessels (arterioles and capillaries) provides a straightforward avenue to realistically explore the relation between microvascular diseases and global systemic hemodynamics. Moreover, the model allows to go in either direction, from reduction techniques to create even simpler 1D models, to 3D models built on top of the 1D skeleton provided by the ADAN model. In a nutshell, this model has become a milestone in the race for new generations of high definition blood flow models capable to aid cutting-edge cardiovascular research.

Acknowledgements

The authors acknowledge the support of the Brazilian agencies CNPq and FAPERJ. Also, the authors acknowledge Dr. Mario Sansuke Watanabe, Dr. Lucas Omar Müller and Dr. Luis Alonso Mansilla Alvarez for their contributions to the development of the activities reported in this article. ●

“ The remarkable feature of the ADAN model is the extremely detailed anatomical description of the arterial network, which enables to tackle, in silico, complex hemodynamic phenomena that remain poorly understood.”

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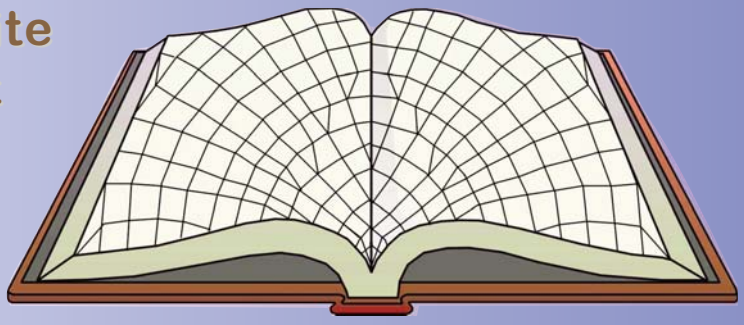
Fundamentals of the Finite Element Method for Heat and Mass Transfer



P. Nithiarasu, R.W. Lewis & K.N. Seetharamu
Wiley, 2016 (2nd edition)

BOOK REVIEW

ISBN: 978-0-470-75625-6, 464 pages, hard cover, $105 (List Price).

Contents: Preface; 1: Introduction; 2: Some Basic Discrete Systems; 3: The Finite Element Method; 4: Steady-State Heat Conduction in One-dimension; 5: Steady-state Heat Conduction in Multi-dimensions; 6: Transient Heat Conduction Analysis; 7: Laminar Convection Heat Transfer; 8: Turbulent Flow and Heat Transfer; 9: Heat Exchangers; 10: Mass Transfer; 11: Convection Heat and Mass Transfer in Porous Media; 12: Solidification; 13: Heat and Mass Transfer in Fuel Cells; 14: An Introduction to Mesh Generation and Adaptive Finite Element Methods; 15: Implementation of Computer Code; References; A: Gaussian Elimination; B: Green's Lemma; C: Integration Formulae; D: Finite Element Assembly Procedure; E: Simplified Form of the Navier–Stokes Equations; F: Calculating Nodal Values of Second Derivatives; Index.

This is the 2nd edition of the book; the 1st edition was published in 2004, also by Wiley, with a slightly different title ("Fluid Flow" instead of "Mass Transfer"). This 2nd edition is an extended version of the original book, and includes, in addition to the more basic material of heat conduction and laminar convection, also heat convection due to turbulent flow, mass transfer, fuel cells, and other advanced topics. The first two authors are well-known authorities on the subject from Swansea University, one of the world leading places in Finite Element Method (FEM) research, and a birth place of the method, strongly associated with the name of the late Olek Zienkiewicz. The third author is a chaired professor from PESIT in Bangalore, India.

According to the Preface, the book is intended for students at various levels, for engineers and for early career researchers. It is well written and easy to read, with a good mixture of theory, applications and numerical examples. Moreover, the book has a very pleasing appearance, and is scattered with many illustrations. It has an excellent structure, which makes it easy for the reader to find what she is looking for. Regarding the content, there is a strong emphasis on the physics and engineering; the computational methods discussed here are presented as tools for the engineer who wishes to solve physical problems, not merely as methods for solving mathematical problems governed by PDEs. Thus, quite a lot of background is provided for the physical problems under study, which adds a very nice touch that is often missing from FE books. Another manifestation of this is the fact that in the examples the parameters are given numerical values and physical units (using the metric system). At the same time, most of the equations are also cast in a non-dimensional form, which introduces important non-dimensional numbers (Reynolds, Rayleigh, Nusselt, etc.). I find that expressing the equations in both dimensional and non-dimensional forms to be an excellent feature. Each chapter ends with exercises and a list of references. The reader may freely download the 2D source code that is used in the book and its documentation from www.zetacomp.com.

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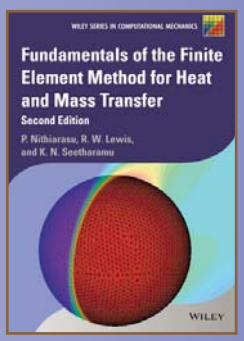

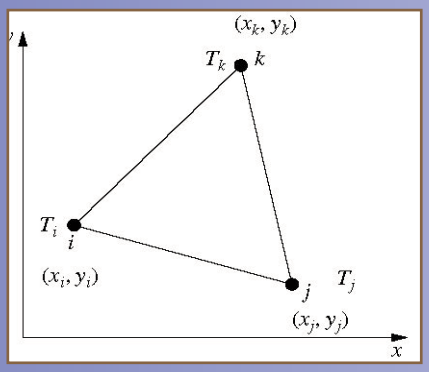

Figure 1:
Naming the nodes of the linear triangular element as i, j and k. This is Figure 3.7 in the book

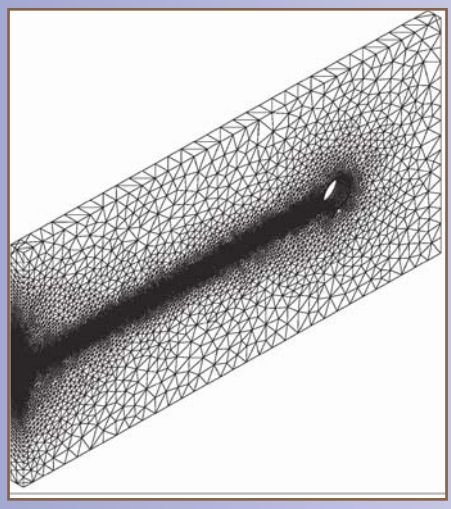

Figure 2:
Mesh used for the problem of turbulent flow over a circular cylinder at Re=10,000. This is Figure 8.10(c) in the book

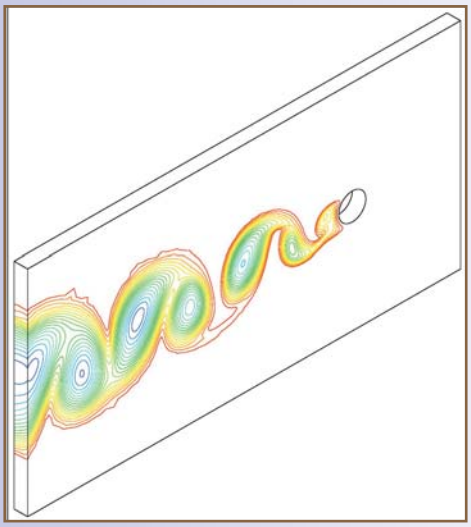

Figure 3:
Snapshot of the solution obtained for the problem of turbulent flow over a circular cylinder at Re=10,000. This is Figure 8.13(a) in the book

The book's style, at least partly, is typical to the classical Swansea style which is liked by many. I confess that there is one feature in this style which I find slightly confusing: this is the naming of element nodes by 'i', 'j', 'k', etc., as in the linear triangular element shown in *Figure 1*. Using this notation, the index i in the shape function N_i does not admit the value 1 or 2 or 3 but signifies the element's node named 'i'. Incidentally, this notation is not used consistently in the book; for example, on p. 184, the index i is used in the standard way, namely i goes from 1 to the number of spatial dimensions, and the summation convention is used. Moreover, while the nodes of the linear triangular element are named i, j and k, the nodes of the quadratic triangular element are numbered from 1 to 6. Having observed this, it is true that generations of students and engineers studied FEM using this notation, apparently without any difficulty.

The book can roughly be divided into 5 parts: the basics (chapters 1-3), heat conduction (chapters 4-6), convective heat transfer (chapters 7 and 8), special advanced topics (chapters 9-13) and FE programming (chapters 14 and 15).

In chapter 1, the laws of heat transfer and basic mathematical models are presented. Chapter 2 discusses systems which are naturally described as discrete to begin with (as opposed to continuous systems which are discretized by an approximation method). Already here some of the basic FE tools make an appearance, like the notion of an 'element' and the assembly operation. The exercises at the end of this chapter relate to varied and interesting physical systems. Chapter 3 covers basic concepts in FE analysis. Three approaches for FEM are described: the Ritz formulation, the Rayleigh-Ritz formulation and the Galerkin formulation, the latter being the most general and receives here, justly, more attention.

Chapter 4 discusses FEM for 1D steady-state heat conduction. In addition to the standrad material, the chapter discusses static condensation, 1D problems in cylindrical coordinates and conduction-convention systems. Chapter 5 extends this to 2D and 3D. Chapter 6 deals with transient heat conduction. Implicit and explicit Euler schemes are discussed. A non-standard topic included here is time-discretization using FEs, where linear shape functions are used in each time-slab.

Chapter 7, dealing with laminar convection, includes very useful non-standard material. First, the Navier-Stokes (NS) equations (for a compressible fluid) are developed in a comprehensive manner. Then a convection-diffusion problem is described. The authors explain the difficulty in solving the convective problem using the standard Galerkin method. Various Petrov-Galerkin methods have come to the rescue in the FE literature. Here, the Characteristic Galerkin (CG) method is presented; it is based on a moving coordinate, so that the convective term disappears from the PDE. For scalar problems this method is identical to Taylor-Galerkin, as Lohner et al. showed in 1984. Next, the Characteristic Based Split (CBS) scheme is presented, for the solution of the NS problem in 2D. As the authors write, the operator splitting "enhances the

pressure stability and allows the use of arbitrary interpolation functions for both velocity and pressure." Mathematically, this means that the Babuska-Brezzi stability condition is satisfied. The authors also show how to modify the CBS scheme to make it fully explicit. Various applications and examples are discussed, among them non-isothermal flows and buoyancy-driven heat transfer.

Chapter 8, which was added in the 2nd edition, deals with heat transfer in a turbulent-flow environment. This is an extremely important and difficult subject. As the authors write, "Despite considerable progress… one has to admit that molecular turbulence is still an unresolved problem and will remain so for several more years." In the following pages, the authors explain the concept of "turbulence models" clearly, as well as notions like time-averaging, Kolmogorov length scale, RANS, κ-ε models, κ-l models, LES, DES, MILES and DNS. Then, the CBS formulation discussed in the previous chapter is used to solve the heat-transfer problem. The method is applied to buoyancy-driven flow, as well as to turbulent flow over a circular cylinder at Re=10,000; see *Figures 2 and 3*. The von-Karman vortex street is clearly observed in *Figure 3*.

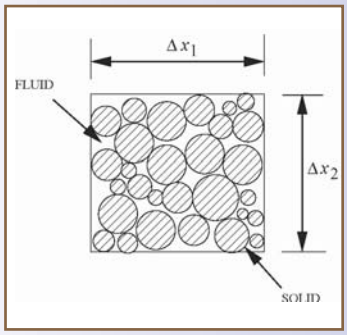

Figure 4:
Fluid saturated porous medium – control volume. This is Figure 11.3 in the book

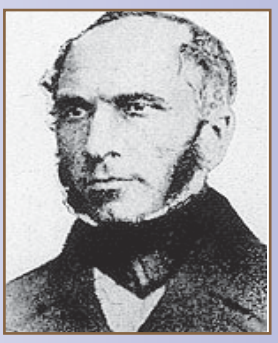

Figure 5:
Henry Darcy, the French engineer who Proposed the Darcy law for flow in porous media, 1856

Chapter 9 discusses practically important systems of heat exchangers. A full and general analysis of these systems requires the solution of the NS equations with turbulence, using the methods discussed previously. However, this chapter proposes shortcuts, using much simpler analysis methods. Chapter 10 deals with mass transfer problems, where the main unknown is the species concentration. Only the isothermal case is considered, in which the problems are analogous to those of heat transfer. Chapter 11 discusses heat and mass transfer in a saturated porous medium (*Figure 4*), and includes a description of some of the pioneering work of Lewis and later of Nithiarasu. The basic governing law is that of Darcy (*Figure 5*), but extended laws are mentioned here too. The computational techniques discussed include the semi-implicit and quasi-implicit schemes. The chapter includes a discussion on non-isothermal flows in porous media, natural convection and the treatment of the interface between a saturated porous medium and a free fluid.

Chapter 12 deals with heat transfer in problems involving a phase change, namely involving both a solid and a liquid. The basic problem is sometimes called the Stefan problem. The authors present the enthalpy formulation, whose advantage is that it does not require any front tracking, and obtains the solution in both the solid and liquid regions "in one shot". Of course, the whole subject is covered here only briefly, since it is very wide and can easily be expanded to an entire book. Chapter 13 covers the subject of fuel cells, which are important electrochemical energy-converting devices.

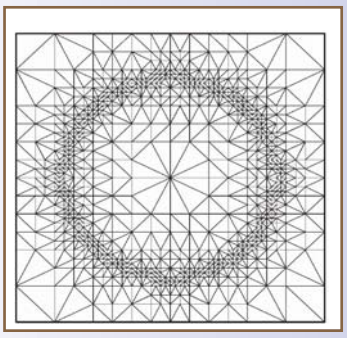

Figure 6:
Delaunay triangulation. This is Figure 14.7(b) in the book

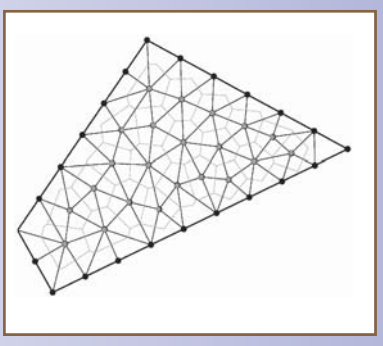

Figure 7:
Centroidal Voronoi Tesselation. This is Figure 14.12(d) in the book

Chapter 14 is a nice introduction to mesh generation and to adaptive FE techniques. Included among the many methods discussed here are Delaunay triangulation *(Figure 6)* and Centroidal Voronoi Tesselation *(Figure 7)*. The sections on adaptivity include a discussion on error estimation, mesh refinement based on the celebrated Zienkiewicz-Zhu scheme and interpolation-based refinement. Chapter 15 describes the open-source Fortran code mentioned above, solving time-dependent heat conduction and convection problems using CBS and time-stepping.

In summary, this is an excellent, well-written book and quite a unique treatment of FE methods for heat and mass transfer. It is highly recommended either as a textbook for students or as a reference book on the subject for practitioners and researchers.

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KSCM 2018 Spring Workshop

KSCM 2018 Spring Workshop was held in Lotte World Tower Signiel Seoul, Korea, on **11 May 2018**. The workshop organized by Korean Society for Computational Mechanics aims to bring together Korean researchers in the field of computational mechanics and encourage research exchange and networking. Five speakers – Maenghyo Cho (Seoul National University), Gihun Son (Sogang University), Yeunwoo Cho (KAIST), Keonwook Kang (Yonsei University), & Junseok Kim (Korea University) – gave lectures on recent research trend in computational mechanics. Further information will be found at: http://www.kscm-society.org/.

Figure 1:
Group Photo of KSCM 2018 Spring Workshop Attendants

Figure 2:
Speakers of KSCM 2018 Spring Workshop: Maenghyo Cho (Seoul National University) and Junseok Kim (Korea University)

1st KSCM-GACM Joint Workshop

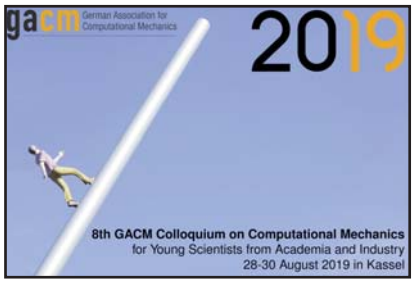
1st KSCM-GACM (German Association for Computational Mechanics) Joint Workshop will be held in Seoul National University, Korea, on **24~25 October 2018**. The main objective of this joint workshop between Korean and Germany is to stimulate and facilitate discussion, interaction, and collaboration in computational mechanics area. 10 German and 15~20 Korean scholars are expected to participate the joint workshop.

Figure 3:
Kick-off meeting to organize 1st NCCMK 2019

1st National Congress of Computational Mechanics of Korea (NCCMK 2019, tentative name)

1st National Congress of Computational Mechanics of Korea (NCCMK 2019, tentative name) will be held in Seoul, Korea, on **14~15 February 2019**. This will be the first national conference organized by KSCM, COSEIK (Computational Structural Engineering Institute of Korea), KSIAM (Korean Society for Industrial and Applied Mathematics), KSCFE (Korean Society for Computational Fluids Engineering), KSME (Korean Society of Mechanical Engineers) CAE & Applied Mechanics division, & KSCE (Korean Society of Civil Engineers) Computational Mechanics division. Further information will be found at: http://www.kscm-society.org/.

8th GACM Colloquium on Computational Mechanics



The 8th GACM colloquium on computational mechanics for young scientists from academia and industry, the colloquium of the German Association on Computational Mechanics (GACM) will be organized on **August 28 - 30, 2019** in documenta city **Kassel, Germany**. The colloquium is hosted by the Institute of Structural Mechanics and the Institute of Mechanics of the University of Kassel. The previous seven conferences of this series were held in Bochum (2005), Munich (2007), Hannover (2009), Dresden (2011), Hamburg (2013), Aachen (2015) and Stuttgart (2017).

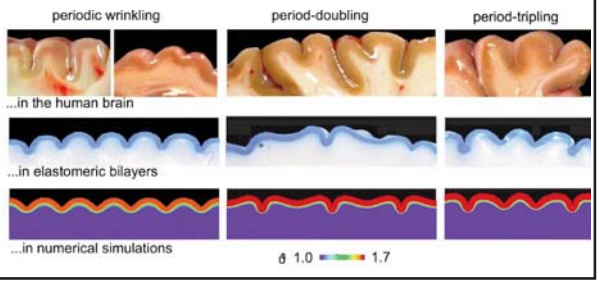
The GACM Colloquium on Computational Mechanics intends to bring together young scientists who are engaged in academic and industrial research on Computational Mechanics and Computer Methods in Applied Sciences. It provides a platform to present and discuss recent results from research efforts and industrial applications. Thematically arranged sessions and organized mini-symposia as well as social events will provide an environment for lively discussions in an informal atmosphere. The contributions from young researchers will be supplemented by plenary lectures from three senior scientist from academia and industry as well as from the GACM Best PhD Award winners 2017 and 2018. In addition, there will be a poster session including a plenary poster-flash. All submitted posters are eligible for the GACM Best Poster Award. Young scientists from Europe and all other continents are welcome to this colloquium. Presentations will be given in English.

GACM Best PhD Awards

It is a great pleasure for us to announce that the outstanding doctoral theses of Dr.-Ing. Silvia Budday is honored with the GACM Best PhD Award 2017. Her thesis on “The Role of Mechanics during Brain Development” was supervised by Prof. Paul Steinmann at the FAU Erlangen-Nürnberg. The award will be handed over on the occasion of the 8th GACM Colloquium on Computational Mechanics in Kassel 2019.

Dr.-Ing. Silvia Budday:
“The Role of Mechanics during Brain Development”

This thesis combines analytical, computational, and experimental analyses to explore the role of mechanics during brain development. After thoroughly characterizing the region-specific constitutive behavior of brain tissue, a mechanical model for brain growth is established using the nonlinear field theories of continuum mechanics, supplemented by the theory of finite growth. The model consists of a morphogenetically growing outer cortex and a stretch-induced growing inner core, combining the two popular but competing hypotheses that cortical folding is either driven by axonal tension or differential growth. Analytical analyses quantify the critical conditions at the onset of folding; numerical simulations additionally predict the highly nonlinear post-buckling behavior and provide new evidence towards the emergence of higher order wrinkling modes. Analytical and computational predictions are experimentally validated using a model system comprised of an elastomeric bilayer. Taken together, this work emphasizes that the key regulators of pattern selection in the developing brain include cortical thickness, brain geometry, stiffness, and growth. The mechanical model explains why larger mammalian brains tend to be more convoluted than smaller brains. Numerical predictions agree well with the classical pathologies of lissencephaly and polymicrogyria and bridge the scales from cellular events on the microscopic level towards form and function on the organ level.



3rd International Conference on Computational Methods

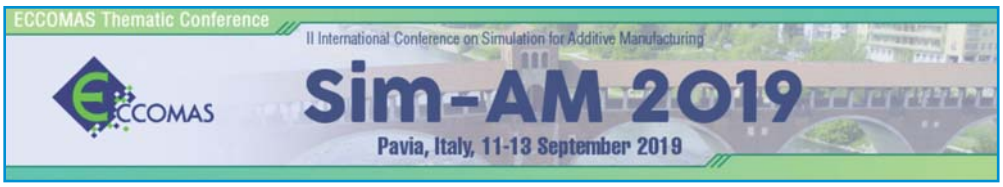
The ICCM is an international conference providing an international forum for exchanging ideas on recent advances in areas related to computational methods, numerical modelling and simulation, as well as their applications in engineering and science. It will accommodate presentations on a wide range of topics to facilitate inter-disciplinary exchange of ideas in science, engineering and related disciplines, and foster various types of academic collaborations.
http://www.sci-en-tech.com/ICCM/index.php/ICCM2018/ICCM2018

12th National Conference of Computational Mechanics and 9th Meeting of the AIMETA Materials Group

The XXII National Conference of Computational Mechanics and the IX Meeting of the AIMETA Materials Group are of interest to all the researchers in the area of applied mechanics, with special regard to solid mechanics, structural mechanics, fluid mechanics, and mechanics of materials. The aim of the conference is to provide a meeting for researchers from different disciplines who are developing and using advanced analytical and numerical methods for the solution of problems of engineering and applied sciences, in order to facilitate the interdisciplinary exchange and dissemination of the most recent developments in the fields of computational mechanics and mechanics of materials.
https://gimc2018.sciencesconf.org/

GIMC GRUPPO MATERIALI AIMETA

The Second International Conference on Simulation for Additive Manufacturing



The Second International Conference on Simulation for Additive Manufacturing (Sim-AM 2019) will be organized in Pavia, Italy, on 11-13 September 2019. Additive manufacturing (AM) is evolving as one of the most promising manufacturing technologies for creating solid structures of virtually any shape. Furthermore, AM allows to produce more complex shapes than those obtained through classical manufacturing techniques. As a consequence, applications for AM products range across many fields in engineering, from design models to lightweight components for automotive or aerospace industry, from patient-specific medical implants to civil engineering structural and/or architectural components.
http://congress.cimne.com/SIM-AM2019/

First Joint Workshop of the German Association

On February 28th and March 1st, 2018 in the beautiful and historic building of the CISM, International Centre of Mechanical Sciences, in Udine, the first joint GACM-GIMC meeting took place, seeing the participation of a group of Italian and German scientists on computational mechanics. The meeting was organized by the current presidents of the two associations, Michael Kaliske (GACM) and Anna Pandolfi (GIMC), as well as by two other members of the GIMC committee, Sonia Marfia and Alessandro Reali. The idea of having a joint meeting came out during the International Conference of Theoretical and Applied Mechanics (ICTAM 2016) with the aim of strengthening the collaborative research activities between Germany and Italy, already characterized by numerous bilateral links and successful productions. The goal of a small but intensive meeting restricted the selection of the participants to the ones really interested in pursuing a collaboration. The choice of the location fell naturally on the CISM in Udine, known to possess great organization capabilities and ideal facilities to host small groups of scientists. During the workshop, a total of 29 participants had the pleasure of listening to a variety of interesting talks concerning innovative and classical topics of computational mechanics.

Here is the scientific program.

Keynote Lecture - **Bernhard Schrefler** (Università di Padova): *"Modeling drug delivery and efficiency in the tumor microenvironment"* (obliged to cancel at the last minute because of a nasty cold)
Keynote Lecture - **Tim Ricken** (Universität Stuttgart): *"Multiscale Simulation of Multiphase Materials"*

Otto von Estorff (TU Hamburg): *"Computational Methods in Acoustics"*
Maria Laura De Bellis (Università del Salento): *"Virtual element formulation for isotropic damage"*
Laura De Lorenzis (TU Braunschweig): *"Phase-field modelling of fatigue fracture"*
Carolin Birk (Universität Duisburg-Essen): *"Polygon elements based on the scaled boundary finite element method and potential applications"*
Carlo Callari (Università del Molise): *"A new algorithm for the tracking of shear failure surfaces based on incompatible modes and strong discontinuity kinematics"*
Steffen Freitag (Ruhr-Universität Bochum): *"Real-time predictions of uncertain settlements in mechanized tunneling"*
Paolo Valvo (Università di Pisa): *"Stress analysis of wind turbine blades based on an extended shear formula"*

Figure 1: *Official picture of the participants to the GACM-GIMC workshop*

and of the Italian Group of Computational Mechanics

Marc-André Keip (Universität Stuttgart): *"Modeling of magnetorheological elastomers across scales: from microstructure evolution to overall stability analysis"*
Stefano Mariani (Politecnico di Milano): *"Micromechanical characterization of polysilicon films through on-chip testing and Bayesian inverse modelling"*
Felix Fritzen (Universität Stuttgart): *"Data-assisted computational homogenization using the RNEXP and open challenges"*
Ferdinando Auricchio (Università di Pavia): *"3D printing: computational issues"*
Stefan Löhnert (Leibniz Universität Hannover): *"Simulating crack face contact and heat transfer across cracks using the XFEM"*
Lorenzo Sanavia *(Università di Padova): "Modelling desiccation cracks in variably saturated porous media within the phase-field approach"*
Detlef Kuhl (Universität Kassel): *"Higher Order Accurate Time Integration Schemes"*
Michele Marino (Università di Roma Tor Vergata and Leibniz Univeritat Hannover): *"Computational mechanical modelling of crimped fibers: a multiscale finite element formulation for flexible composites"*
Udo Nackenhorst (Leibniz Universität Hannover): *"Computational Biomechanics of Bones"*
Giuseppe Vairo (Università di Roma Tor Vergata): *"Chemo-mechano-biological modelling of soft tissues: the case of aortic tissues via a multiphysics and multiscale approach"*
Peter Betsch (Karlsruher Institut für Technologie): *"GENERIC-based numerical methods for coupled thermomechanical problems"*
Fabian Duddeck (TU München): *"Multi-fidelity optimization using physical and mathematical surrogates"*
Elio Sacco (Università di Cassino e del Lazio Meridionale): *"Homogenization of nonlinear composites based on FTA approach"*

Figure 2: *Organizers of the workshop (from left): Anna Pandolfi, Alessandro Reali, Sonia Marfia and Michael Kaliske*

All the presentations were at a very high level and they brought out interesting discussions. The scientific program was topped off by a wonderful social dinner in the Trattoria ai Frati with delicious Italian food and drinks and time for further interesting conversation. Given the success of the initiative, GACM and GIMC want to regularly repeat it on a two or three-year basis. More information on the workshop can be found at **http://www.cism.it/courses/E1802/** ●

Anna Pandolfi
&
Michael Kaliske

Figure 3: *Historical conference room at the CISM building*

JSCES Autumn School 2017 on Nonlinear Finite Element Method for Elastoplastic Analysis

A three-day course entitled “JSCES Autumn School 2017 on Nonlinear Finite Element Method for Elastoplastic Analysis” was held during October 4-6, 2017, at Arata Hall in Joining and Welding Research Institute, Osaka University. The aims of this course are to promote the spread of fundamental and up-to-date technologies of nonlinear finite element method for solids and structures, and to support engineers, of Things) and a review of PSE studies.

On the second day of the worksh

During this camp, 6 keynote speakers gave talks about their research backgrounds; also 18 students presented their ongoing researches.

The best presentation awards were given to two students *(Figure 6)*.

All attendees enjoyed exchanging their experience and idea in a beautiful late summer atmosphere *(Figure 7)*. ●

by: Yuichi Shintaku

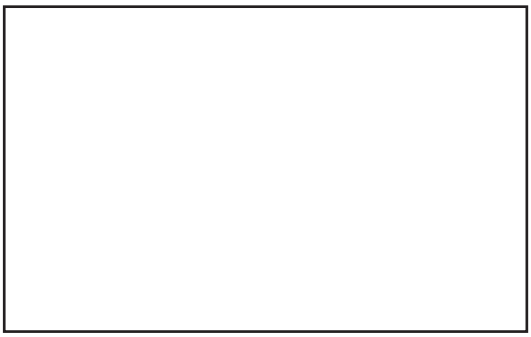


Figure 1: Lecture by Prof. Kenjiro Terada (Tohoku Univ., President of JSCES)

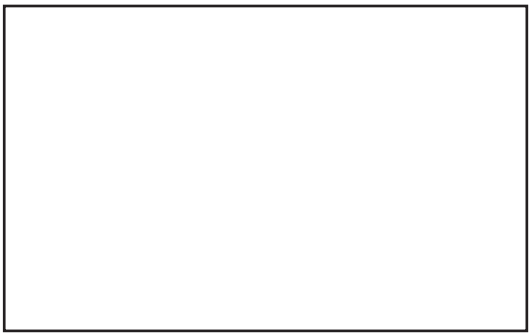
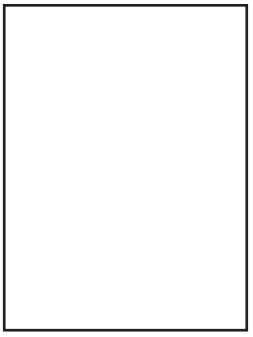


Figure 2: A view of a lecture in the summer school



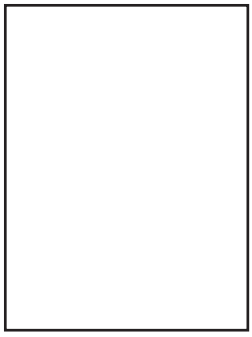


Figure 3: *Special guest lectures: Profs. T.J.R. Hughes & T.E. Tezduyar*

5 June

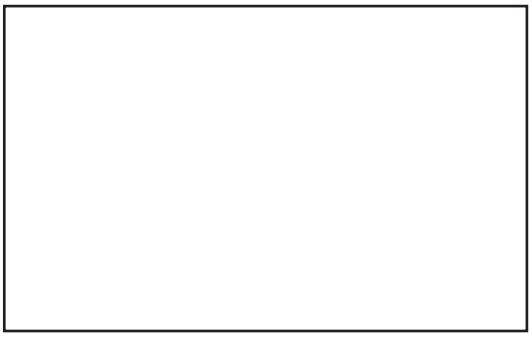


Figure 4:
Prof. Zheng-Ming Sheng presents his keynote speech

Figure 5:
Workshop tour following Alan M. Turing and

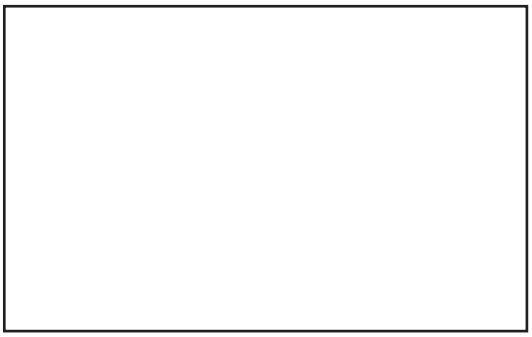


Figure 6:
Winners of the best presentation awards
Mr. Keita Imai (left) and Mr. Naoto Harasawa, Prof. Takahiro Yamada, Vice-president of JSCES (center)

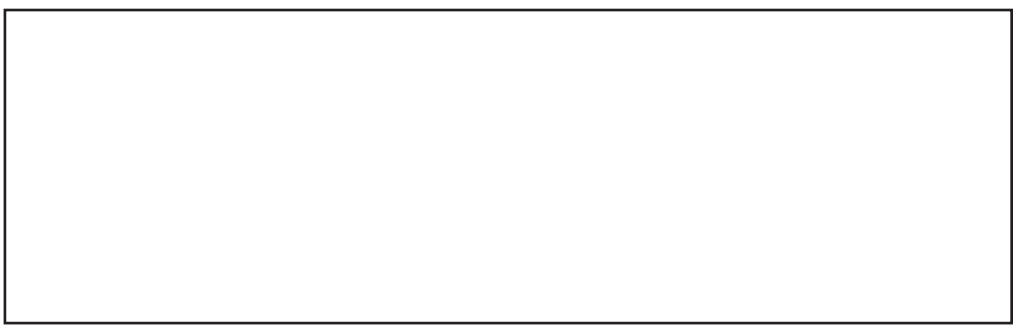


Figure 7:
Participants of the JSCES summer camp 2017

For all inclusions under ***JACM*** *news please contact:*
Hiroshi Okada
hokada@rs.noda.tus.ac.jp

The Japan Association for Computational Mechanics (JACM) elected a new executive council in March 2018. After three years as president of JACM, Professor Shinobu Yoshimura, The University of Tokyo, left the board. The new executive council members for 2018-2021 are as follows:

President:
Professor Hiroshi Okada, Tokyo University of Science
hokada@rs.noda.tus.ac.jp,
http://www.rs.noda.sut.ac.jp/me/laboratories/okada_laboratory.html

Vice Presidents:
Professor Seiya Hagihara, Saga University
hagihara@me.saga-u.ac.jp, http://research.dl.saga-u.ac.jp/souran_profile/en.d42663754dcf613b59c123490551be02.html

Professor Hiroshi Okuda, The University of Tokyo, okuda@k.u-tokyo.ac.jp,
https://www.k.u-tokyo.ac.jp/pros-e/person/hiroshi_okuda/hiroshi_okuda.htm

Secretary General:
Professor Ryuji Shioya, Toyo University
shioya@toyo.jp, http://www2.toyo.ac.jp/~shioya/shioya.html

Figure 1:
Hiroshi Okada
President

Figure 2:
Seiya Hagihara
Vice President

Figure 3:
Hiroshi Okuda
Vice President

Figure 4:
Ryuji Shioya
Secretary General

JACM is a loosely coupled umbrella organization covering 29 computational mechanics related academic/industrial societies in Japan through communication with e-mail and web page (http://www.sim.gsic.titech.ac.jp/jacm/index-e.html). The number of individual members is about 310. In the election for the president, the general council members representing the participating societies voted.

JACM took a part of the Seventh Computational Mechanics Symposium held on December 7, 2017. The symposium is organized by the Science Council of Japan (SCJ) in association with eight computational mechanics related academic societies in Japan. The function of SCJ is defined as “The Science Council of Japan was established in 1949 as a “special organization” under the justification of the Prime Minister, operating independently of the government for the purpose of promoting and enhancing the field of science, and having science reflected in and permeated in administration, industries and people’s lives. It represents Japan’s scientists both domestically and internationally …” (http://www.scj.go.jp/en/scj/index.html). The annual SCJ Computational Mechanics Symposium has become a new tradition and is an evidence of how Japanese science and engineering community finds computational mechanics to be a very important area.

In the seventh symposium, eight young researchers representing the participating computational mechanics related societies presented their latest research outcomes. They are basically recent recipients of Young Investigators Award of each society. Dr. Masaya Suzuki of JAXA (Japan Aerospace Exploration Agency) participated the symposium as the recipient of JACM Young Investigators Award. The other societies participated are: “Japan Society for Computational Methods in Engineering (JASCOME)”, “CAE Konwakai”, “The Computational Mechanics Division of The Japan Society of Mechanical Engineers (CMD, JSME)”, “Japan Society for Computational Engineering and Science (JSCES)”, “The Japan Society for Simulation Technology (JSST)”, “The Visualization Society of Japan (VSJ)” and “The Japan Society for Industrial and Applied Mathematics (JSIAM)”.

Figures 5:
Speakers of 7th Computational Mechanics Symposium

On March 20, a symposium cerebrating the 20th anniversary of “ADVENTURE Project” was held on the campus of The University of Tokyo. JACM cosponsored the symposium. The “ADVENTURE” stands for “ADVanced ENgineering analysis Tool for Ultra large REal world”. “ADVENTURE Project” was initiated in 1997 as one of five projects in the "Computational Science & Engineering" field selected by the "Research for the Future (RFTF)" program sponsored by the Japan Society for the Promotion of Science (JSPS). The “ADVENTURE Project” was initiated and has been led by Professor Shinobu Yoshimura of The University of Tokyo.

The “ADVENTURE Project” has developed an advanced general-purpose open source computational mechanics system for large-scale analysis and design named "ADVENTURE" towards Petascale and Exascale computing. According to the Web Page of the “ADVENTURE Project” (http://adventure.sys.t.u-tokyo.ac.jp/), due to its excellent performance in solving ultra-large scale mechanics problems together with its open source strategy, the ADVENTURE system is now being used by a variety of industrial and academic groups. Around 9,700 users from various industries, universities, and research centers have registered. Around 9,700 users from various industries,universities, and research centers have registered. To date, over 43,000 modules have been downloaded free of charge. A private company developed and released a commercial version of the software called ADVENTURECluster, which has been installed in various companies, universities and national laboratories.

The symposium started with speeches by Professor Shinobu Yoshimura and Professor Genki Yagawa (past president of IACM). Presentations on the latest developments of the ADVENTURE System by the key members of the project followed. ●

Figures 6 & 7:
Professors Shinobu Yoshimura and Genki Yagawa at the ADVENTURE Project 20th Anniversary Symposium.

Central European Association for Computational Mechanics

The CEACM has gone the long way since its initiation by prominent scientists, Herbert Mang, former President of ECCOMAS and Ivo Babuska, a Gauss-Newton medalist of IACM. In the present configuration, CEACM counts the following Central European countries (in alphabetical order): Austria, Bosnia and Herzegovina, Croatia, Czech Republic, Hungary, Poland, Slovakia and Slovenia. In 2017, CEACM has voted new Statutes of the Association and has elected a new Executive Committee that consists of the President, Bernhard Pichler, the Vice-President, Adnan Ibrahimbegovic and the Past-President, Pavel Polach.

The scientific activities of CEACM in 2017 concern organizing two short courses and a scientific conference.

The first short course was organized in Budapest, July 3-7, 2017.
The course, entitled "PARAMeters UNCertainties Uncertainty Quantification, Parameter Identification, and Challenges in Engineering Computations" (URL: https://www.wire.tu-bs.de/paramunc/), was jointly organized by two Hungarian institutions: Institute for Computer Science and Control (SZTAKI) and Budapest University of Technology and Economics, in collaboration with CVUT Prague, TU Braunschweig and UT Compiegne. The course lecturers were: Dr. Noémi Friedman (TUBs), Prof. Adnan Ibrahimbegovic (UTC), Prof. Hermann G. Matthies (TUBs), Dr. Habib N. Najm (Sandia Nat. Lab.), Dr. Elmar Zander (TUBs), Dr. Gergely Vígh, (BME), Dr. Mihály Weiner (BME). The topics addressed in the course were related to both general theoretical background of uncertainty quantification in parameter identification and to optional specialized topics from different fields selected from the plenary lectures of the last-day course workshop. Among the participants who attended the course, the vast majority were doctoral students from different CEACM countries, along with a couple of participants from industry.

The second short course was organized in Ljubljana, September 17-19, 2019.
The course entitled "Current Research on Solids & Fluids: Computations, FE Code Coupling, Model Reduction, Probability…" (URL: http://www.eccomas-msf-2017.eu/), was jointly organized by University of Ljubljana, University of Rijeka, TU Braunschweig and UT Compiegne. The course lecturers were: Prof. Adnan Ibrahimbegovic (UTC), Prof. Hermann G. Matthies (TUBs), Prof. Nikolaos Limnios (UTC), Prof. Abdellatif Ouahsine (UTC), Prof. Jose-Luis Perez Aparicio (UPV),

Figure 1: *ECCOMAS MSF 2017 Conference: course lecturers and participants*

Prof. Florian deVuyst (UTC). The main objective of this course was to provide graduate students and researchers with an extensive review of numerical models for computational solid and fluid mechanics, and pertinent modern developments in model reduction, probability aspects and uncertainty quantification. It presented the current state-of-the-art in finite element, finite volume and discrete element modeling of nonlinear problems in solid and fluid mechanics, and their coupling with thermal, electric and magnetic fields and their interactions. The course participants (see photo 1) were doctoral students from CEACM and other European countries, along with a couple participants from North America.

In 2017, CEACM sponsored a scientific conference ECCOMAS MSF 2017 – Multiscale Computational Methods for Solids and Fluids, which was held in Ljubljana, September 20-22, 2017. This was the 3rd conference in series organized by Adnan Ibrahimbegovic, this time in collaboration with Bostjan Brank and Ivica Kozar, which attracted close to hundred scientific presentations, with the contributing authors coming from 32 different countries. The ECCOMAS MSF 2017 Proceedings are available for download at the conference website (URL: http://www.eccomas-msf-2017.eu/). The conference provided a platform for exchange among leading specialists in analysis and design of complex engineering structures and systems, coming from aerospace, civil and mechanical engineering, material science, and in the design and analysis of numerical algorithms from applied mathematics. The main goal was elaborating the multi-field and multi-physics approach, which has significantly modified previously firm frontiers among these traditional engineering disciplines. The introductory plenary lectures of each day of this conference were scheduled to set the contents and the boundaries as well as indicate the main issues concerning computational methods for multi-scale analysis in solid and fluid mechanics. The plenary speakers were: Prof. Hermann Matthies, TU Braunschweig, Germany, Prof. Pierre Ladeveze, ENS-Cachan, France, Prof. Bernhard Schrefler, Univ. Pavia, Italy and Prof. Adnan Ibrahimbegovic, TU-Compiegne, France (see photo 2). A number of keynote lectures and organized sessions (containing 4-6 papers) were also scheduled at the conference. The organized sessions concerned: Aging of construction materials, Thermomechanical coupling, Electromagnetic-mechanics coupling, Uncertainty Propagation, Fluid-structure interaction, Multi-phase flows, Stochastic Processes, Structural Mechanics. ●

Figure 2:
ECCOMAS MSF 2017 Conference: plenary lecturers at conference banquet

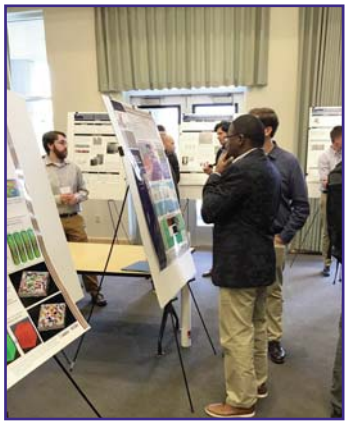
The The U S Association for Computational Mechanics has been active in holding thematic conferences, organized by various Technical Thrust Areas (TTAs). Below are summaries of the most recent ones and plans for future meetings.

Recent Advances in Integrated Computational and Experimental Methods for Additive Manufacturing
Golden, Colorado - September 6-8, 2017

Conference Website: http://aicem-am2017.usacm.org/

Figure 1: *Lecture being given on campus of Colorado School of Mines*

Figure 2: *Discussions taking place at poster session*



A thematic conference held as part of the USACM Technical Thrust Area on Manufacturing and Materials Processing and co-sponsored by the Mineral, Metals, and Materials Society (TMS), the goal of this conference was to bring together researchers from both the computational mechanics and materials science research communities involved in advancing the state-of-the-art in process modeling of additively manufactured (AM) materials and structures. A theme of the conference was integration of computational modeling and experiment, leveraging the unique manufacturing aspects of AM, to improve overall modeling predictivity and to enable process optimization.

Additive manufacturing (AM) holds the promise of revolutionizing current paradigms in engineering design, manufacturing, and material and structural performance. To fully realize the possibilities of AM requires significant advances in both the process and performance modeling of additively manufactured materials and structures. The modeling and simulation of AM processes is multidisciplinary in nature, involving multiple physics as well as multiple time and space scales, thus requiring interdisciplinary research efforts. The unique manufacturing process of AM affords the possibility of tightly integrating in-situ measurements and computational modeling.

The conference was organized by Joseph Bishop (Sandia National Laboratories), Amy Clarke (Colorado School of Mines, TMS) and Gregory Wagner (Northwestern University). Taking place at the Green Center on the beautiful Colorado School of Mines campus, the conference featured 31 talks and 15 posters by graduate students and post-doctoral fellows. Financial support for some travel was provided by Sandia National Laboratories and the National Science Foundation. ●

Minimum Residual & Least-Squares Finite Element Methods
Portland, Oregon - October 2-4, 2017

Conference Website: https://sites.google.com/pdx.edu/dpg/home

This USACM Workshop in Portland, OR, brought together global researchers working on Least-Squares Finite Element Methods, Discontinuous Petrov Galerkin Methods, and other emerging methods built around residual minimization properties. The workshop was part of the TTA on Mathematical Methods in Computational Engineering & Sciences.

It was the third in a series of workshops with the same goal. The first workshop in this series was held in Austin, Texas, in 2013. The second workshop was held in Delft, The Netherlands, in 2015.

The third edition in Portland was organized by Jay Gopalakrishnan (PSU) and received partial support from Portland State University. The scientific committee was comprised of Zhigqiang Cai (Purdue University); Leszek Demkowicz (The University of Texas at Austin); Norbert Heuer (Pontificia Universidad Catolica de Chile), and Rob Stevenson (University of Amsterdam). The workshop began with an informal social gathering at the organizer's house. The workshop atmosphere was vibrant with 30 speakers pushing the frontiers of our mathematical understanding of residual minimization methods. There were 40 registered participants. While US participants formed the majority of, participants joined also from Chile, China, France, Germany, and The Netherlands. The workshop concluded with a walk across Portland's

Figure 3:
Participants gathering in front of the science museum

newest bridge and a guided tour of a submarine moored in the Willamette river.

The program with titles of all 30 talks may be found at https://sites.google.com/pdx.edu/dpg/program. Abstracts are also available on the conference website. ●

Nonlocal Methods in Fracture
Austin, Texas - January 15-16, 2018

Nonlocality, which has a long history in continuum mechanics, is gaining importance in simulation of fracture. It is a feature of multiple contemporary approaches to fracture modeling, including peridynamics and certain implementations of fracture in finite element codes. For example, phase field methods for fracture implicitly include a length scale, implying a connection with nonlocality. However, researchers in this spectrum of techniques often fail to agree on the proper role of nonlocality in modeling fracture, including disagreement on whether nonlocality has any justifiable physical basis, or whether instead it should be viewed as an artificial way of regularizing the mathematical model. This workshop was organised to encourage better understanding of nonlocality among practitioners of different techniques for fracture modeling and identify common ground and differences between its role in various methods. This forum promoted better communication among researchers and an improved understanding of the strengths and challenges in different computational methods involving aspects of nonlocality.

Organized by Michael Borden (Brigham Young University), John Foster (University of Texas at Austin), Chad Landis (University of Texas at Austin), Rob Lipton (Louisiana State University), Erdogan Madenci (University of Arizona), Pablo Seleson (Oak Ridge National Laboratory), and Stewart Silling (Sandia National Laboratories), the conference took place at the AT&T Conference Center on the University of Texas campus. Over 22 talks were presented, with ample time for discussion scheduled into the program. A conference dinner in downtown Austin provided an informal setting for more discussions.

Support from Oak Ridge National Laboratory is gratefully acknowledged. ●

Figure 4:
Informal gathering during reception at conference on UT-Austin campus

Figure 5:
Break during the conference at the AT&T Center

USACM Upcoming Events
further details at usacm.org

- **Workshop on Meshfree and Particle Methods: Application and Theory**
  *Santa Fe, New Mexico, September 10-12, 2018; **http://mfpm2018.usacm.org/***
- **IGA 2018: Integrating Design and Analysis**
  *Austin, Texas; October 10-12, 2018; **http://iga2018.usacm.org/***
- **Uncertainty Quantification in Computational Solid and Structural Materials Modeling,**
  *Baltimore, Maryland, January 17-18, 2019; **http://uq-materials2019.usacm.org/***
- **Toplology Optimization Roundtable**
  *Albuquerque, New Mexico, March 10-13, 2019; **https://erolunal.com/dev/workshop/***
- **15th U.S. National Congress on Computational Mechanics**
  *Austin, Texas, July 28-August 1, 2019; see **http://www.usacm.org/** for more details.* ●

CSMA Prizes:

Every year CSMA rewards the best two PhD thesis of the year. For the 2017 edition, the CSMA prize committee has examined 24 applications. The two awardees are Alexis FAURE and Liang MENG. Liang MENG is designated as the CSMA candidate for the ECCOMAS award for the best PhD theses in 2017.

Alexis FAURE: ***Shape optimization and architectured structures of materials by level-set method taking into account interfaces with graded properties***
Advisors: R. Estevez (Université Joseph Fourier, Grenoble), R. Parry (INP Grenoble)

Figure 1:
Alexis FAURE

Shape optimization methods are promising methods and are gradually becoming industrialized. They provide the ability to automatically design structures with optimal behavior. They are outstanding tools for exploration and design of new materials. We use these methods to generate architectured multi-phased materials with prescribed thermoelastic properties. We first propose several solutions and we classify them by the mechanisms they rely on in order to control the effective properties. We also propose to evaluate the influence of an interface with a gradient of properties on the obtained architectures. Eventually we focus on the plausible manufacturing solution to produce our architectured materials. In this context, additive manufacturing methods (often considered as the support of an incoming industrial revolution) is our main option. We introduce several strategies to circumvent some limitations and side effects of these manufacturing methods during optimization process. We particularly focus on Fiber Deposition Molding, which induce an important mechanical anisotropy in processed parts. Then we consider the problem of overhanging features in design and propose a way to handle them prior to additive manufacturing using a mechanical criteria. Finally we take into account geometrical non linearities in optimization process. We highlight the pros and cons of this new modeling by presenting several applications of nonlinear actuators design.
Current situation: Alexis Faure is Research Engineer at SIMaP laboratory Grenoble

Liang MENG: ***Reduced Shape-space Approach to Material Characterization***
Advisors: P. Breitkopf (Université des Technologies de Compiègne), B. Raghavan, INSA Rennes

Figure 2:
Liang MENG

The thesis lies at the intersection of three disciplines: numerical methods, experimental techniques, and machine learning. The primary aim of this work is to develop a group of algorithms for characterization by inverse analysis of a material's constitutive law. In the field of material characterization, indentation test is especially attractive since it is considered non-destructive, and may be performed even on a structure in service. However, the inverse problem based solely on this curve tends to be ill-posed, leading to non unique identification solution, i.e., the "mystical material pair", for whom the corresponding force-displacement curves are almost identical despite the very different material properties. The basic idea is then to complete the identification process with innovative experimental measurements, such as the laser microscope, which allows measuring the 3D residual imprint after the withdrawal of the indenter. To address the advantage of this measured over P-h curve, we propose to construct, within a reduced affine space, a manifold of shapes admissible to the postulated constitutive law, experimental and simulation setups, based on synthetic data. The intrinsic dimensionality of the manifold limits the number of identifiable parameters allowing validating numerically the experimental procedures. Considering both the model and measurement errors, we develop a series of local manifold learning algorithms to solve the inverse problem iteratively.
Current situation: Liang MENG is Assistant Professor, Northwestern Polytechnical University, Xi'an, Chine
CSMA selected the PhD thesis of Liang MENG for the ECCOMAS Olympiads 2018

Creation of the CSMA Juniors section:
objectives and first achievements

The French Computational Structural Mechanics Association (CSMA) encouraged and launched in 2016 its section of young researchers, called CSMA Juniors. The range of actions of this section is large, but the main objectives are to facilitate exchanges and collaborations among the young generation (under 40) of CSMA, to propose scientific activities which are useful and unique for young researchers, and to help CSMA in its activities (such as social networking) and promote these to young researchers. The section is driven by a committee made of 9 members, which is renewed by half every two years.

A major activity of the section is the organization of an annual two-day workshop dedicated to the young generation of CSMA (including PhD students, post-docs, and junior researchers with permanent position), even though the participation of more experienced researchers to this event and the connection between juniors and seniors is highly supported. For its first edition in May 2017, the workshop was connected to the French National Congress on Computational Structural Mechanics (organized every 2 years by CSMA in the beautiful Giens peninsula on the French Riviera); the workshop was thus considered as an extension of the CSMA congress, and this will be the case in each odd year. In March 2018, the second edition of the CSMA Juniors workshop was organized in a CNRS center near Paris and was sponsored by the industrialist group SAFRAN.

During these two first editions, the workshop gathered between 60 and 80 attendees with invited people (CSMA PhD prize awardees for instance). Many sessions with innovative formats were proposed, such as:

- short courses on specific topics (these are selected from plenary lectures and mini-symposia of the CSMA congress in odd years), given by and for young scientists, and with both theoretical and practical sessions;
- hackathon (software competition);
- classes on key numerical tools (Python, Paraview, GIT, …);
- exchange with academic and industrialist seniors on the construction of scientific careers, the link between industry and academia, or job opportunities;
- poster or short (3 min) talks sessions;
- practical session on writing a research paper.

The annual workshop, as well as all other activities carried out by the CSMA Juniors section, are evidence of the dynamism of the CSMA association. They constitute rich and useful means to help young CSMA members acquire experience and develop their research career, in addition to feeling fully involved in the life of CSMA. ●

Ludovic Chamoin
President of the CSMA Juniors Committee

Figure 3:
Hackathon session during the 2017 workshop

Figure 4:
group picture during the 2018 workshop

After 20 years of spontaneous collaborations between several research groups on computational mechanics from Germany and Brazil, and with the intention of creating a more intense and permanent cooperation in the field, the 1st German-Brazilian Workshop on Computational Mechanics (GBWCM) was held on February 19-20, 2018, at the University of São Paulo, Brazil. This was an initiative from researchers of both countries and was promoted by the Polytechnic School of the University of São Paulo together with the Brazilian Association for Computational Methods in Engineering (ABMEC) and the Deutsche Forschungsgemeinschaft (DFG). The event was a tremendous success, with talks from over 40 invited speakers from both countries, and over 200 pre-registered participants (at no cost) in the audience. Many prominent figures from the German and Brazilian scenes were present. A few pictures of the event are displayed below (more at the workshop´s photo gallery https://www.flickr.com/photos/poliusp/albums/72157690622125772).

The workshop consisted of oral presentations followed by group discussions on a great variety of topics covering several branches of computational mechanics. In the social side, a welcome lunch was held on the eve of the event at very pleasing restaurant nearby the university campus, where the guests were greeted with dishes from our local cuisine and shots of the Brazilian national drink, caipirinha. Also, on February 16, a visit to the São Paulo´s Sambadrome was organized, to watch the Carnival 2018 Champion´s Parade. More details on this fruitful event can be found at https://www.gbwcm2018.com. The 2nd German-Brazilian Workshop on Computational Mechanics is planned to happen in 2019 in Germany, possibly in Essen. The tentative dates are September 5-6, 2019. This is to be announced soon.

In addition to the report of the 1st GBWCM, ABMEC is pleased to reinforce the announcement for the 39th Ibero-Latin-American Congress on Computational Methods in Engineering (XXXIX CILAMCE), which will be held in Paris, France, November 11-14, 2018. CILAMCE is the main event promoted ABMEC, and this year is being jointly organized by the Université de Technologie de Compiègne, the Sorbonne Universites and the University of São Paulo, under the lead of Prof. Adnan Ibrahimbegovic (IUF/Sorbonne/UT-Compiégne) as chairman, and Prof. Paulo Pimenta (University of São Paulo) as co-chairman. The congress activities will take place at the UT-Compiègne campus (in Compiègne), as well

Figure 1:
1st GBWCM. Invited speakers gather at the end of the workshop for a joint picture before leaving for a last caipirinha

Figure 2:
1st GBWCM. Opening Ceremony: Prof. Eduardo M. B. Campello, ABMEC´s president, welcomes all participants

Figure 3:
Profs. Paulo Pimenta, Jörg Schröder and Peter Wriggers discuss at the main board after the national anthems of both countries

Figure 4:
1st GBWCM. Prof. Peter Wriggers giving his talk

Figure 5:
1st GBWCM. Participants

as at the historical building of the École Polytechnique (in Quartier Latin, Paris). A very nice social program is also being offered. This will be the first time, since its inception in 1977, that CILAMCE will be held outside Brazil, Argentina, Portugal, Italy or Spain. We are very excited for this innovation and opportunity. More details and updated information can be found at https://cilamce2018.rbv.utc.fr.
We invite all IACM members and enthusiasts of computational mechanics to participate in the 39th edition of our CILAMCE series of congresses.
Hope to see you there!

Warmest regards,
Prof. Eduardo M. B. Campello
(University of São Paulo), ABMEC President
Prof. Felício B. Barros
(Federal University of Minas Gerais), ABMEC Vice-President

39th CILAMCE – Ibero-Latin-American Congress on Computational Methods in Engineering

Paris

November 11-14, 2018

Chair: Prof. Adnan Ibrahimbegovic (IUF/Sorbonne/UTC)
Co-chair: Paulo Pimenta (USP)

SORBONNE UNIVERSITÉS utc Université de Technologie Compiègne USP

conference diary planner

01 - 05 July 2018	**ACE-X2018 – 12th Int. Conference on Advanced Computational Engineering & Experimenting**		
	Venue: Amsterdam, The Netherlands	*Contact:*	www.acex-conference.com
02 - 06 July 2018	**ESMC 2018 - The 10th European Solid Mechanics Conference**		
	Venue: Bologna, Italy	*Contact:*	www.esmc2018.org
11 - 15 July 2018	**ECCM VI - 6th European Conference on Computational Mechanics**		
	Venue: Glasgow, U.K.	*Contact:*	www.eccm-ecfd2018.org
11 - 15 July 2018	**ECFD VII - 7th European Conference on Computational Fluid Dynamics**		
	Venue: Glasgow, U.K.	*Contact:*	www.eccm-ecfd2018.org
22 - 27 July 2018	**WCCM-XIII - PANACM-II : 13th World Congress on Computational Mechanics** jointly organized with the **2nd Pan American Congress on Computational Mechanics**		
	Venue: New York, USA	*Contact:*	http://www.wccm2018.org/
5 - 7 Sept. 2018	**ICOMP'18 - 3rd Int. Conference on Computational methods in Manufacturing Processes**		
	Venue: Barcelona, Spain	*Contact:*	https://icomp18.sciencesconf.org/
17 - 21 Sept. 2018	**AMWPS 2018 - 2nd Int.Conference on Advanced Modelling of Wave Propagation in Solids**		
	Venue: Prague, Czech Republic	*Contact:*	*http://www.ceacm.org/*
10 - 12 Oct. 2018	**IGA2018 - Isogeometric Analysis**		
	Venue: Austin, Texas, USA	*Contact:*	http://congress.cimne.com
6 - 9 Nov. 2018	**MECOM 2018 - XII Argentine Congress on Computational Mechanics**		
	Venue: Tucuman, Argentina	*Contact:*	www.facet.unt.edu.ar/mecom2018
11 - 14 Nov. 2018	**39th CILAMCE – Ibero-Latin-American Congress on Computational Methods in Engineering**		
	Venue: Paris, France	*Contact:*	https://cilamce2018.rbv.utc.fr
13 - 16 Jan. 2019	**KomPlas Tech 2019 - Conference on Computer Methods in Materials Technolog**		
	Venue: Zakopane, Poland	*Contact:*	http://www.eccomas.org
25 - 27 May 2019	**ADMOS IX - International Conference on Adaptive Modeling and Simulation**		
	Venue: Campello (Alicante), Spain	*Contact:*	http://congress.cimne.com
3 - 5 June 2019	**COUPLED PROBLEMS -VIII Int. Conference on Coupled Problems in Science & Engineering**		
	Venue: Barcelona, Spain	*Contact:*	http://congress.cimne.com/coupled2019/
12 - 14 June 2019	**CFRAC - 6th Int. Conf. on Computational Modeling of Fracture & Failure of Materials & Structures**		
	Venue: Braunschwei, Germany	*Contact:*	http://congress.cimne.com/cfrac2019
24 - 26 June 2019	**COMPDYN - 7th Int. Conf. on Computational Methods in Structural Dynamics & Earthquake Engineering**		
	Venue: Creta, Greece	*Contact:*	https://2019.compdyn.org
24 - 26 June 2019	**UNCECOMP - 3rd Int. Conf. on Uncertainty Quantification in Computational Sciences & Engineering**		
	Venue: Creta, Greece	*Contact:*	https://2019.uncecomp.org/
8 - 12 Sept. 2019	**SMART 2019 - 8th Conference on Smart Structures and Materials**		
	Venue: Paris, France	*Contact*:	http://www.eccomas.org
15 - 18 July 2019	**MULTIBODY 2019 - Multibody Dynamics**		
	Venue: Duisburg, Germany	*Contact:*	http://www.eccomas.org
1 - 6 Sept. 2019	**YIC 2019 - Eccomas Young Investigators Conference**		
	Venue: Cracow, Poland	*Contact:*	http://www.ptmkm.pl/pl/node/134
5 - 7 Sept 2019	**COMPLAS 2019 - XIV International Conference on Computational Plasticity**		
	Venue: Barcelona, Spain	*Contact:*	http://congress.cimne.com/complas2019/
8 - 12 Sept. 2019	**PCM-CMM 2019 - 4th Polish Congress of Mechanics & 23rd International Conference on Computer Methods in Mechanics**		
	Venue: Krakow, Poland	*Contact:*	http://pcm-cmm2019.com/
18 - 21 Dec. 2019	**APCOM 2019 - 7th Asian Pacific Congress on Computational Mechanics**		
	Venue: Taipei, Taiwan	*Contact:*	http://www.apcom2019.org/
19 - 24 July 2020	**ECCOMAS CONGRESS 2020** jointly organized with the **WCCM XIV - 14th World Congress on Computational Mechanics (IACM)**		
	Venue: Paris, France	*Contact:*	http://www.eccomas.org/