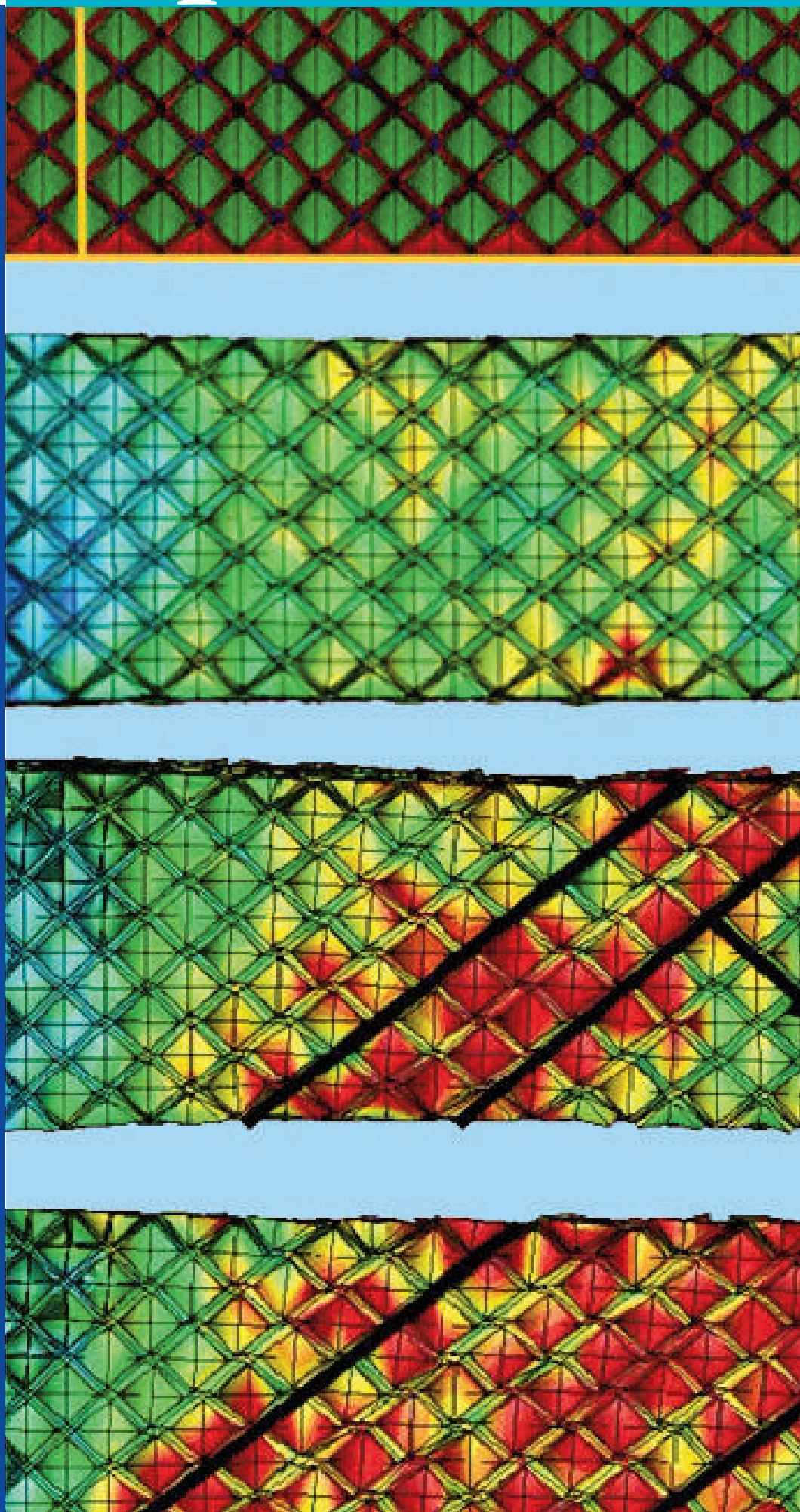
iacm expressions



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contents

editorial

High Performing Computing (HPC) is typically understood by the general public as the computer solution of challenging and outstanding problems with exceptional requirements in terms of size, CPU time and data storage, using big and expensive supercomputing machines equipped with state of the art parallel computing technology. HPC services have been so far mostly provided by specialized national or regional governmental organizations that host such powerful computers and are responsible for distributing their supercomputing capacity among users under request.

This approach to HPC has resulted in the use of HPC facilities mostly for research purposes in selected scientific areas. As an example, HPC is commonly used for the solution of complex problems in computational physics and chemistry, such as weather prediction, ADN studies and molecular dynamics simulations, just to name a few.

The benefits of using HPC for engineering applica-tions are well understood by companies and many initiatives for promoting HPC in industry have been launched by the competent administrations. However, despite much effort and money invested, the fact is that, with few exceptions, the use of centralized or in-house supercomputing facilities by industry is very limited or null. For instance, while large automotive and aerospace companies have been using HPC simulation for some time, most smaller enterprises in these and other engineering sectors are much less experienced. Without the infrastructure and expertise to configure and manage a HPC cluster, or the strive for interacting with a HPC service provider, the barrier to entry can be too large, which discourages companies, and also many research organizations, from taking the first step to invest in a new technology.

My vision is that cloud computing may rapidly change the current HPC paradigm. Cloud computing offers organizations a cost-effective platform to expand their computing capacity, or a way of trying HPC on-demand before bringing a cluster in-house. Cloud computing can also be used to provide burst capacity for users equipped with a HPC system. This relates not only to flexibility on their current computing capacity, but also the ability to scale the number of software licenses an organization is using.

Cloud computing services are already offered by different providers and their use simplifies every day, as commercial software companies offer cloud computing as an option for using thecodes via innovative SaaS and CaaS (software/computing as a service) modes. These new computing services will surely have an impact in the very near future on how research and industrial organizations will choose to adopt cloud computing, continue to invest in on premise hardware, or continue using the centralized supercomputing infrastructures.

A note on recent IACM activities. The 13th World Congress on Computational Mechanics (WCCM) held on 22-27 July 2018 in the city of New York was a full success with some 3500 participants from all over the world attending the gathering jointly organized with the 2nd Pan American Congress on Computational Mechanics. Congratulations to Prof Jacob Fish from Columbia University and his team for an excellent organization of the congress.

The New York congress was also the occasion for the renewal of several IACM officers of the Executive Council of the IACM, as listed on page 2 of this bulletin. Congratulations and best of luck to the new IACM president Prof Antonio Huerta (Technical University of Catalonia, Barcelona, Spain) and many thanks to the IACM officers stepping down from their positions for their work, in particular the past IACM president Prof Wing Kam Liu (Northwestern University, US).

The countdown for WCCM 2021 in Paris has already started and this promises to be another landmark IACM event that will be held jointly with the large ECCOMAS 2020 congress (wccm- eccomas2020.org). I also advise to keep an eye on the different events regularly promoted by the IACM in different countries.

Eugenio Oñate
Editor of IACM Expressions

To the IACM Community: @ IACM Community

"In 1986 the first World Congress of the Association took place in Austin, Texas, and at the same meeting the first Executive Council was elected." This was the first sentence of the Editorial letter from O.C. Zienkiewicz in the 1st issue of the IACM Expressions in Spring 1996. Since 1986 the International Association of Computational Mechanics has made a great stride to promote and consolidate our community all over the world. Today IACM is a well-established professional society, with almost five thousand affiliates worldwide. Credit for these achievements must go for the past-presidents and officers of IACM who generously devoted precious time to the society and also to each individual member working everyday for the success and impact of computational mechanics. ***Thank you all!***

Consequently, I am humbled and very enthusiastic to serve as the President of such an outstanding association, leading an Executive Council composed of brilliant scientists and friends. Our primary mission is to stimulate and promote education, research and practice in Computational Mechanics, to foster the interchange of ideas among the various fields contributing to this science, and to provide forums and meetings for the dissemination of knowledge. We will keep the hard work in the rapidly changing environment. Of course, the major events at the core of the Association will remain our World Congresses (Paris 2020 & Yokohama 2022) and our IACM Conferences (FEF Chicago 2019) but also, every activity developed by our affiliated associations and members. I encourage you to participate and help the congress organizers hosting minisymposia of your interest!

We are privileged to collaborate with a remarkable network of affiliated associations. As of today, thirty-one societies covering every world region. Their activities and continuous work allow to promote Computational Mechanics in academia, industry, the society at large and, very important, into the new and young generation of researchers and engineers.

While we have achieved great things, there is much more to do. Working to build the future, we count very much on the interaction and collaboration with every member and also, notably, with our esteemed international affiliated societies.

Together we will succeed.

Antonio Huerta
President of IACM

Probabilistic Machine Learning for the Small-Data Challenge in Computational Science

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Usual big data and small volume of data associated with expensive large computational models

Machine learning is revolved around empirical models such as kernels or Neural Networks (NN) that require big data and efficient algorithms for their identification and training. If the volume of data is not sufficiently large, it may not generally be possible to train the NN to the desired behavior. In the framework of computational science and engineering, while computationally taxing simulations are typically used to generate big data, the quantities of interest (QoI) from each such simulations are typically much smaller. In many such problems, however, and in particular in the context of uncertainty quantification (UQ), the fundamental challenge is in characterizing the map from input to QoI in a manner that is conducive to inference and design.

In these problems, a large number of expensive function evaluations are required in order to explore, sufficiently well, both the design and the input sets. The size of the former set depends on the range of design variables while the latter reflects uncertainty in input variables. While these problems are best classified under the heading of “small data”, they share some of the conceptual and computational challenges of “big data” with further complications pertaining to scarcity of evidence, and the necessity to extract the most knowledge, with quantifiable confidence, from scarce data.

Role played by statistical and probabilistic learning methods for stochastic computational models

In this context, probabilistic learning is a way for improving the knowledge that one has from only a small number of expensive evaluations of a computational model in order to be able to solve a problem, such as a nonconvex optimization problem under uncertainties with nonlinear constraints, for which a large number of expensive evaluations would be required, which, in general, is not possible.

This is one reason for which statistical and probabilistic learning methods have been extensively developed (see for instance, [1-10]) and play an increasingly important role in computational physics and engineering science [11]. In large scale model-driven design optimization under uncertainty, and more generally, in artificial intelligence for extracting information from big data, statistical learning methods have been developed in the form of surrogate models that can easily be evaluated [12-14] such as, Gaussian process surrogate models [15,16], Bayesian calibration methods [17-19], active learning [20,22], which allow for decreasing the numerical cost of the evaluations of expensive functions. This is particularly crucial for the evaluation of expensive stochastic functions induced by the presence of a probabilistic modeling of uncertainties in large computational models. This is a major challenge that requires the use of suitable mathematical methods and algorithms such as, for instance, those proposed in [23-26].

A novel probabilistic learning on manifolds

This very short paper deals with the presentation of a novel probabilistic learning on manifolds that can be viewed as a computational statistics tool for addressing challenging problems based on large scale simulations in the presence of model uncertainties. We present the main idea and illustrations of this novel probabilistic learning on manifolds, recently developed [27-29], which provides a mathematical framework and algorithms to address difficult problems such as those encountered for data driven and optimization problems using expensive large numerical models [30] (in presence of uncertainties generated by modeling errors [31] or due to random media [32,33]), but also for enhancing the predictability of large computational models of very complex systems, such as those related to combustion in hypersonic flows [34].

Representing the random response of the given stochastic computational model.
We consider a stochastic computational model of a discretized complex system for

which its response is written as $\mathbf{Q} = \mathbf{f}(\mathbf{W},\mathbf{U})$ in which $\mathbf{W}$ is a vector-valued random parameter controlling the system, with values in a given admissible set C_w, whose probability distribution $P_{\mathbf{W}}(d\mathbf{w})$ is given and has C_w as support. In the computational model, the probabilistic model of uncertainties is represented by the vector-valued random parameter $\mathbf{U}$ for which the probability distribution $P_{\mathbf{U}}(d\mathbf{u})$ is given and is independent of $\mathbf{W}$. The quantities of interest are described by the vector-valued random variable $\mathbf{Q}$ that is a deterministic nonlinear transformation $\mathbf{f}$ of $\mathbf{W}$ and $\mathbf{U}$. The mapping $\mathbf{f}$ represents the response $\mathbf{q} = \mathbf{f}(\mathbf{w},\mathbf{u})$ of the computational model for given $\mathbf{u}$ and given $\mathbf{w}$ in C_w. It is assumed that the probability distribution of the random vector $\mathbf{X} = (\mathbf{W},\mathbf{Q}) = (\mathbf{W}, \mathbf{f}(\mathbf{W},\mathbf{U}))$ has a density with respect to $d\mathbf{x}$.

Constructing the initial dataset using the expensive stochastic computational model, objective, and fundamental difficulties. An initial dataset of length N (with N small) is constructed as the set of N points $\{\mathbf{x}^{d,j}, j=1,\ldots,N\}$ with $\mathbf{x}^{d,j} = (\mathbf{w}^{d,j}, \mathbf{q}^{d,j})$ in which $\mathbf{q}^{d,j} = \mathbf{f}(\mathbf{w}^{d,j}, \mathbf{u}^{d,j})$ are N independent realizations of $\mathbf{Q}$ (calculated using the expensive computational model) and where $\mathbf{w}^{d,j}$ and $\mathbf{u}^{d,j}$ are N independent realizations of $\mathbf{W}$ and $\mathbf{U}$. Consequently, $\{\mathbf{x}^{d,j}, j=1,\ldots,N\}$ are N independent realizations of random vector $\mathbf{X} = (\mathbf{W},\mathbf{Q})$. Knowing only this initial dataset, the objective is to construct, for any $\mathbf{w}$ in C_w, an estimate $\mathbf{h}^{(N)}(\mathbf{w})$ of $\mathbf{h}(\mathbf{w})$ that is defined, for instance, by $\mathbf{h}(\mathbf{w}) = E\{\mathbf{H}(\mathbf{Q})|\mathbf{W} = \mathbf{w}\}$ in which E is the conditional mathematical expectation given $\mathbf{W} = \mathbf{w}$ and where $\mathbf{H}$ is a given deterministic mapping (for instance, $\mathbf{h}(\mathbf{w})$ could be the objective function of an optimization problem for which $\mathbf{w}$ would be the design parameter belonging to C_w). If each evaluation $\mathbf{q}^{d,j}$ is computationally expensive, then N will be, generally, not sufficiently large for obtaining a good convergence of $\mathbf{h}^{(N)}(\mathbf{w})$ towards $\mathbf{h}(\mathbf{w})$. One way for circumventing this difficulty is to use the probabilistic learning on manifolds that allows for generating $M >> N$ additional realizations $\{(\mathbf{w}^{a,j}, \mathbf{q}^{a,j}), j=1,\ldots,M\}$ without using the expensive computational model in order to construct a better estimate of the conditional expectation that is required for computing $\mathbf{h}^{(N)}(\mathbf{w})$, as shown in [30].

*Probabilistic learning on manifolds [*27]. Given an initial dataset $\{\mathbf{x}^{d,j}, j=1,\ldots,N\}$ of random vector $\mathbf{X}$, the probabilistic learning on manifolds allows for constructing M additional independent realizations $\{\mathbf{x}^{a,j}, j=1,\ldots,M\}$ of $\mathbf{X}$ whose non-Gaussian probability distribution (which is unknown) is assumed to admit a probability density function (pdf) with respect to the measure $d\mathbf{x}$, and assumed to be concentrated in an unknown subset of the set of values of $\mathbf{X}$. In the framework of the previous paragraph, such a concentration of the probability distribution of $\mathbf{X}$ is related to the fact that $\mathbf{X}$ represents the random graph $(\mathbf{W}, \mathbf{f}(\mathbf{W},\mathbf{U}))$ (random manifold). The method proposed allows for generating $\{\mathbf{x}^{a,j}, j=1,\ldots,M\}$ in preserving the concentration and consequently, by avoiding the scattering of the generated additional realizations. The main steps of the construction can be summarized as follows:

(i) A principal component analysis of random vector $\mathbf{X}$ is performed using only the initial dataset $\{\mathbf{x}^{d,j}, j=1,\ldots,N\}$. A new random vector $\mathbf{Y}$ is then constructed for which the realizations $\{\mathbf{y}^{d,j}, j=1,\ldots,N\}$ are directly deduced from $\{\mathbf{x}^{d,j}, j=1,\ldots,N\}$. This step allows for normalizing the initial dataset. It should be noted that the components of $\mathbf{Y}$, which are centered and uncorrelated, are statistically dependent because $\mathbf{Y}$ is not Gaussian. The probabilistic learning on manifolds proposed consists in exploiting this statistical dependence as information for improving the knowledge with respect to the classical statistical methods (for a Gaussian random vector, the uncorrelated components would be independent and so, the random vector would be completely defined, no learning would be required).

(ii) A modification [35] of the multidimensional kernel density estimation method [36] is used for constructing an estimate $p_{\mathbf{Y}}$ of the pdf of $\mathbf{Y}$ using initial dataset $\{\mathbf{y}^{d,j}, j=1,\ldots,N\}$. Estimate $p_{\mathbf{Y}}$ of the pdf of $\mathbf{Y}$ depends on N. A random matrix $[\mathbf{Y}]$ is introduced such that its N columns are made up of N independent copies of random vector $\mathbf{Y}$. The pdf $p_{[\mathbf{Y}]}$ of random matrix $[\mathbf{Y}]$ with respect to $d[\mathbf{y}]$ is then directly deduced from pdf $p_{\mathbf{Y}}$ with respect to $d\mathbf{y}$. A realization of random matrix $[\mathbf{Y}]$ is the deterministic matrix $[\mathbf{y}^d] = [\mathbf{y}^{d,1} \ldots \mathbf{y}^{d,N}]$.

(iii) A Markov chain Monte Carlo (MCMC) generator for $[\mathbf{Y}]$ is constructed [37] in the class of Hamiltonian Monte Carlo methods [37,38], solving a nonlinear Itô Stochastic Differential Equation (ISDE) corresponding to a stochastic

" a novel probabilistic learning on manifolds that can be viewed as a computational statistics tool for addressing challenging problems based on large scale simulations in the presence of model uncertainties."

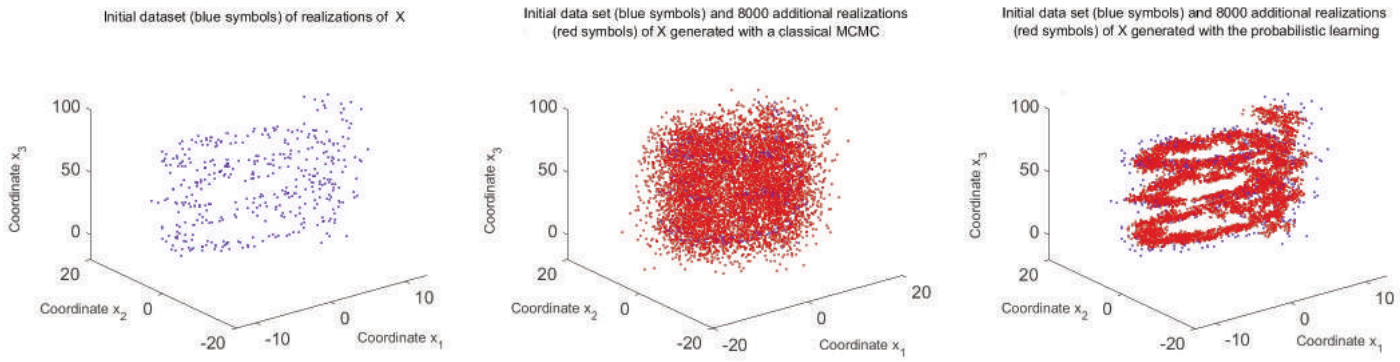


Figure 1:*(from [27])*
Left figure: N= 400 points (blue symbols) of the initial dataset.
Central figure: M = 8,000 additional realizations (red symbols) generated with a classical MCMC algorithm.
Right figure: M= 8,000 additional realizations generated with the probabilistic learning on manifold (red symbols)

nonlinear dissipative Hamiltonian dynamical system, for which $p_{[Y]}([\mathbf{y}])\, d[\mathbf{y}]$ is the unique invariant measure.

(iv) A diffusion-maps approach [39] is used for discovering and for characterizing the local geometry structure of initial dataset $\{\mathbf{y}^{d,j}, j=1,\ldots,N\}$. A diffusion-maps basis is defined as the eigenvectors $[g] = [\mathbf{g}^1 \ldots \mathbf{g}^m]$ associated with the first $m < N$ positive eigenvalues (ordered in decreasing order) of the transition matrix of the Markov chain constructed on $\{\mathbf{y}^{d,j}, j=1,\ldots,N\}$.

(v) A reduced-order representation $[\mathbf{Y}] = [\mathbf{Z}]\,[g]^T$ is introduced in which the new reduced-order random matrix $[\mathbf{Z}]$ has only m columns. The hyperparameter $m << N$, which corresponds to a statistical reduction of $[\mathbf{Y}]$ with respect to data dimension N, must be carefully chosen [29] in order to separate the scales existing in data. Such a separation allows for preserving the concentration of the additional realizations generated by the probabilistic learning and then for avoiding the scattering of generated additional realizations.

(vi) The additional realizations are then obtained by solving the reduced ISDE obtained by projecting the ISDE introduced in step (iii) on the basis $[g]^T$. The invariant measure of this reduced ISDE is the probability distribution of random matrix $[\mathbf{Z}]$.

(vii) The last step consists in analyzing the convergence of the probabilistic learning with respect to N. This point is very important. For a given application, N is imposed and is related to the CPU time that is available. The probabilistic learning algorithm is then applied for several increasing values of the length of the initial dataset: $2 < N_1 < N_2 < \ldots < N_n = N$. The convergence of the sequence of the statistical quantity of interest indexed by $k = 1,\ldots,n$ is then studied. If a convergence is obtained for k less than or equal to n, then the probabilistic learning is converged. If not, length N has to be increased and additional calculations have to be carried out using the expensive stochastic computational model in order to increase length N of the initial dataset.

Illustration of the loss of concentration using a classical MCMC generator and of the efficiency of the probabilistic learning on manifolds that preserves the concentration and avoids the scattering.
Figure 1-(left) displays N= 400 given points of the initial dataset for which the realizations of the random variable $\mathbf{X} = (X_1, X_2, X_3)$ are concentrated around a helical. *Figure 1-(central)* shows M = 8,000 additional realizations of $\mathbf{X}$ generated with a classical MCMC algorithm for which the invariant measure is constructed as explained in step (ii). The concentration is lost and there is a scattering of the generated realizations. *Figure 1-(right)* shows M= 8,000 additional realizations of $\mathbf{X}$ generated with the probabilistic learning on manifold (steps (i) to (vi)) using the reduced ISDE with m = 4. It can be seen that the concentration is kept and there is no scattering of the additional realizations.

Applications

Nonconvex optimization under uncertainties using a limited number of function evaluations [30]. We consider the following nonconvex optimization problem: find the optimal value $\mathbf{w}^{opt}$ that minimizes the objective function $J(\mathbf{w})$ for $\mathbf{w} = (w_1, w_2)$

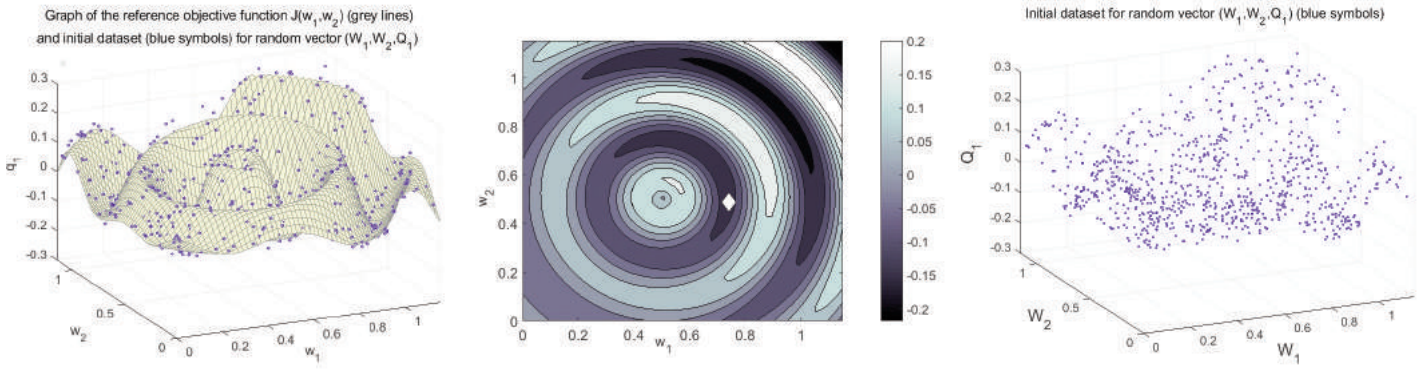


Figure 2:*(from [30])*
*Left figure: graph of the reference objective function J(**w**) (grey lines)*
*Central figure: contour plot of the reference objective function J(**w**) and optimal solution* $\mathbf{w}^{opt} = (w_1^{opt}, w_2^{opt})$ *(white diamond)*
Right figure: initial dataset of the N= 900 realizations $\{(\mathbf{w}^{d,j}, q_1^{d,j}),\ j = 1, \ldots, N\}$ *corresponding to the random variable* $(\mathbf{W}, Q_1)$ *in which* Q_1 *is* J *(blue symbols);*
these points are also surperimposed to the graph of the reference objective function in the left figure

belonging to the admissible set C_w and under the constraints $\mathbf{c}(\mathbf{w}) = (c_1(\mathbf{w}), c_2(\mathbf{w}), c_3(\mathbf{w}), c_4(\mathbf{w})) < 0$ (which means $c_k(\mathbf{w}) < 0$). The computational model is stochastic, depending of a random vector $\mathbf{U}$. The design parameter $\mathbf{w}$ is modeled by a random vector $\mathbf{W} = (W_1, W_2)$ with a given prior probability distribution that is used for generating N points in C_w: $\{\mathbf{w}^{d,j},\ j = 1,\ldots,N\}$. Objective function and constraint vector are written as conditional mathematical expectation $J(\mathbf{w}) = E\{J \mid \mathbf{W} = \mathbf{w}\}$ and $\mathbf{c}(\mathbf{w}) = E\{\boldsymbol{B} \mid \mathbf{W} = \mathbf{w}\}$ in which the random vector $\mathbf{Q} = (J, \boldsymbol{B})$ is the quantity of interest that is constructed as observations of the stochastic computational model. We can then introduce $\mathbf{h}(\mathbf{w}) = (J(\mathbf{w}), \mathbf{c}(\mathbf{w})) = E\{\mathbf{Q} \mid \mathbf{W} = \mathbf{w}\}$. The dimension of $\mathbf{Q}$ is then 5 and the dimension of random vector $\mathbf{X} = (\mathbf{W},\mathbf{Q})$ is 7. The reference model, $(J(\mathbf{w}), \mathbf{c}(\mathbf{w}))$, and the stochastic computational model, $\mathbf{Q} = \mathbf{f}(\mathbf{W},\mathbf{U})$, are known. The graph of the reference objective function $J(\mathbf{w})$ is displayed in *Figure 2-(left)* (grey lines in the left figure). Each component $c_k(\mathbf{w})$ of the reference constraint function $\mathbf{c}(\mathbf{w})$ is a plan in 3D space (c_k, w_1, w_2). *Figure 2-(central)* displays the contour plot of the reference objective function $J(\mathbf{w})$ and shows the location of the optimal solution $\mathbf{w}^{opt} = (w_1^{opt}, w_2^{opt})$ with $w_1^{opt} = 0.74$ and $w_2^{opt} = 0.49$ for which the four constraints are active (the reference solution would not be the same without the constraints) and $J(\mathbf{w}^{opt}) = -0.123$. The initial dataset is made up of N= 900 realizations $\{\mathbf{x}^{d,j} = (\mathbf{w}^{d,j}, \mathbf{q}^{d,j}),\ j = 1, \ldots, N\}$ of random variable $\mathbf{X} = (\mathbf{W},\mathbf{Q})$, which are calculated with the stochastic computational model.

Figure 2-(right) displays the points $\{(\mathbf{w}^{d,j}, \mathbf{q}_1^{d,j}),\ j = 1, \ldots, N\}$ corresponding to the random variable $(\mathbf{W},\mathbf{Q}_1)$ in which $\mathbf{Q}_1$ is the random variable J. These points are also surperimposed to the graph of the reference objective function in *Figure 2-(left)*. The four figures that would illustrate the N realizations of the four random variables $(\mathbf{W},Q_k)$ in which Q_k represents the random variable B_k (the constraints) are not displayed for limiting the number of figures.

The probabilistic learning on manifolds is applied using the initial dataset made up of N = 900 points, with m = 5, for M = 9,000 additional realizations, and M = 90,000 additional realizations, which are used for estimating $(J(\mathbf{w}),\mathbf{c}(\mathbf{w})) = E\{\mathbf{Q} \mid \mathbf{W} = \mathbf{w}\}$ (without using the stochastic computational model). The optimization algorithm that is used is the grid search algorithm. *Figure 3-(left)* shows the contour plot of the objective function estimated with N = 900 points of the initial dataset; the optimal solution cannot be identified because the cost function is not well represented. *Figure 3-(central)* and *Figure 3-(right)* show the contour plots of the objective function estimated with M = 9,000 and M = 90,000 additional realizations using the probabilistic learning on manifolds; the objective function is well represented and therefore, the optimal solution (white diamond) is correctly estimated (white disk) for these two values of M. It can be seen that the probabilistic learning on manifolds allows for reconstructing the contour plot (central and right figures) of the objective function without using the stochastic computational model, but using only the initial dataset. In opposite, the contour plot of the objective function is not correctly reconstructed using only the initial dataset (left figure) and consequently, does not allow for identifying the optimal solution. For M = 9,000, the estimation of the optimal solution is $w_1^{opt} = 0.70$ and $w_2^{opt} = 0.49$ with $J(\mathbf{w}^{opt}) = -0.112$, which is good enough.

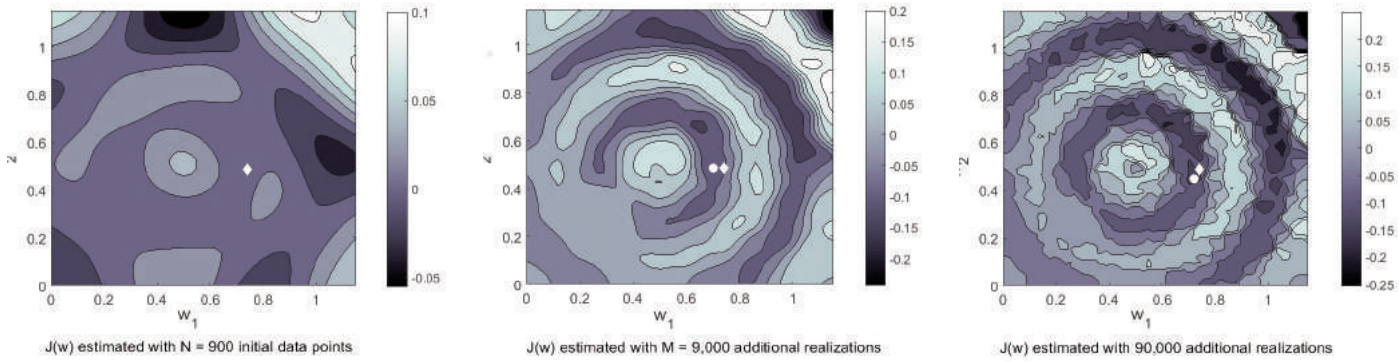


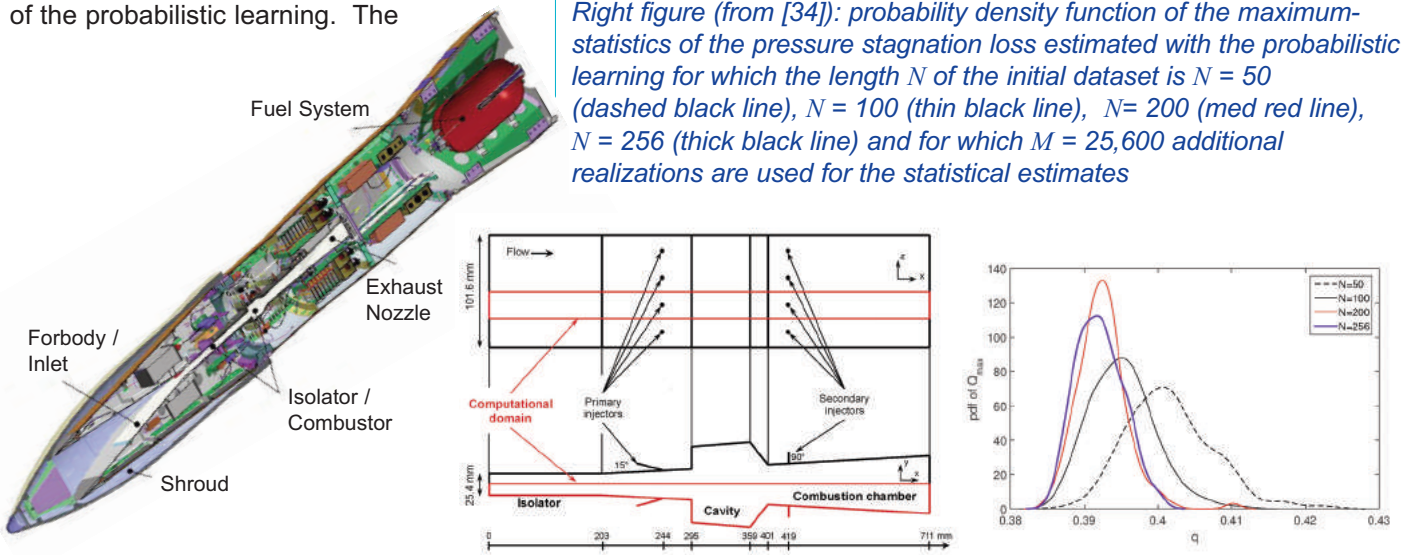
Figure 3:
(from [30]) Left figure: Contour plot of the objective function estimated with N = 900 points of the initial dataset
Central figure: with M = 9,000 additional realizations
Right figure: and with M = 90,000 additional realizations
The reference optimal solution is the represented by the white diamond and the estimated optimal solution using the probabilistic learning on manifolds is represented by the white disk

Enhancing model predictability using the probabilistic learning on manifolds.
We refer the reader to a very interesting challenging application [34] devoted to the analysis of a complex flow inside a scramjet for which the probabilistic learning on manifolds allows for enhancing the predictability of this very complex system that is represented by a large scale computational fluid dynamics model devoted to the combustion in an internal hypersonic flow, which requires to solve the fully-coupled conservation equations of mass, momentum, total-energy, and species for a chemically reacting flow, in taking into account high Reynolds number, high-pressure, real-gas and/or liquid conditions, detailed thermodynamics, and transport processes at the molecular level.

The probability density functions of the quantities of interest and their associated maximum statistics are estimated even though the number of large scale simulations available from the LES runs is not sufficient to obtain sufficiently converged estimates of these quantities. It is shown how the probabilistic learning method learns as a function of the size of the datasets. This type of analysis also serves to determine if the dimension of the initial dataset is sufficiently large for providing an assessment of the quality of the probabilistic learning. The analysis of these probability density functions allows for proposing reasonable interpretations of the physical behavior of the complex turbulent flow in relationship to the mesh size of the fluid domain and the time averaging that is used for constructing the quantities of interest, such as the turbulent kinetic energy at different stream wise locations of the flow (see [34] for the detailed analysis). *In Figure 4*, the three figures are from [34]. The right figure displays the pdf of the maximum statistics of the pressure stagnation loss estimated with the probabilistic learning for which the length N of the initial dataset is N = 50 (dashed black line), N = 100 (thin

" probabilistic learning method learns as a function of the size of the datasets."

Figure 4:
Left figure (from [40,34]: HIFiRE (Hypersonic International Flight Research and Experimentation) Flight 2 payload
Central figure (from [41,42,34]: HDCR (HIFiRE Direct Connect Rig) experimental setup and schematic of the full computational domain
Right figure (from [34]): probability density function of the maximum-statistics of the pressure stagnation loss estimated with the probabilistic learning for which the length N of the initial dataset is N = 50 (dashed black line), N = 100 (thin black line), N= 200 (med red line), N = 256 (thick black line) and for which M = 25,600 additional realizations are used for the statistical estimates



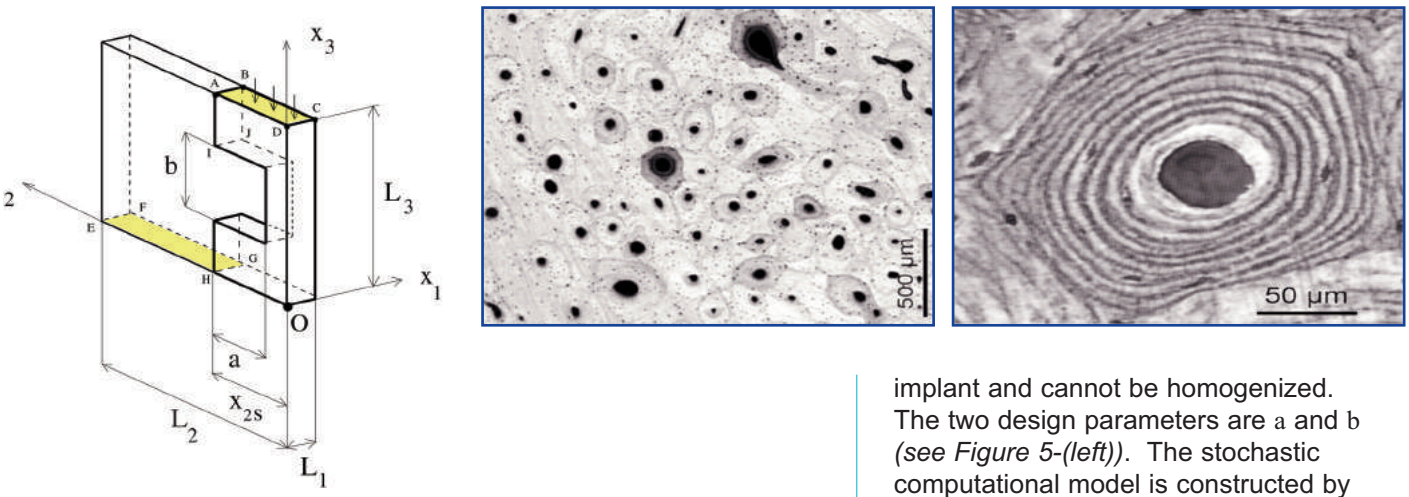


Figure 5 *(from [33])*
Left figure: Parameterization of the geometry for the Tinanium implant occupying domain of the right part of the scheme with $L_1 = 10^{-4}$ m, $L_2 = L_3 = 10^{-3}$ m, and $x_{2s} = 0.4 \times 10^{-3}$ m, in a biological tissue (cortical bone) occupying domain of the left part of the scheme. Central and right figures: Microstructure of the cortical bone at scale 5×10^{-4} m (central figure) and one osteon at scale 5×10^{-5} m (right figure) [Photo from Julius Wolff Institute, harité - Universitatsmedizin Berlin]

black line), N = 200 (med red line), N = 256 (thick black line) and for which M = 25,600 additional realizations are used for the statistical estimates. This figure shows the convergence of the learning when the length N of the initial dataset increases.

Probabilistic learning on manifolds used for solving nonconvex optimization problem related to a large scale stochastic computational model. We refer again the reader to another very interesting challenging application [33] devoted to the design optimization under uncertainties of a mesoscale Titanium implant in a biological tissue using the probabilistic learning on manifolds for solving the nonconvex optimization problem related to the design optimization. The parameterization of the geometry of the Titanium implant in the biological tissue is defined in *Figure 5-(left)*. The scale of the implant is at mesoscale ($L_1 = 10^{-4}$ m, $L_2 = L_3 = 10^{-3}$ m, $x_{2s} = 0.4 \times 10^{-3}$ m), which means that the statistical fluctuations in the biological tissue interact with the implant and cannot be homogenized. The two design parameters are a and b *(see Figure 5-(left))*. The stochastic computational model is constructed by using the finite element discretization of the stochastic linear static boundary value problem for which:

(i) the elasticity field of the cortical bone (heterogeneous linear elastic random medium) is modeled by a non-Gaussian tensor-valued random field controlled by three spatial correlation lengths and by a dispersion coefficient controlling the statistical fluctuations in the anisotropic class,
(ii) the Titanium is a homogeneous linear elastic medium,
(iii) a random static load is applied to the Titanium implant (upper yellow surface in *Figure 5-(left))*, and
(iv) a part of the boundary of the biological tissue is fixed (lower yellow surface in *Figure 5-(left)*.

The spatial correlation lengths and the dispersion coefficient have been identified by solving a statistical inverse problem [43] using measurements [44] performed by a digital image correlation technique. The design optimization consists in minimizing random normal stresses applied to the interface between the implant and the cortical bone. Nonlinear constraints (inequalities) are taken into account in the optimization problem for limiting random shear stresses and random Von Mises stresses in certain regions of the biological tissue. Computation has been performed with a 512 Go-RAM Linux work station using parallel computing with 40 workers (cores). The construction of the reference optimal solution (without probabilistic learning) has required 2,560 hours of CPU time (64 hours of elapsed time) while the construction of the optimal solution using the probabilistic learning on manifolds has only required 104 hours of CPU time (2.6 hours of elapsed time) yielding a gain factor that is about 25. ●

"The design optimization consists in minimizing random normal stresses applied to the interface between the implant and the cortical bone."

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The Finite Cell Method:
An immersed boundary technique for integration of geometric models and numerical analysis

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Geometric surface models describing thin-walled structures are very often defined by NURBS or similar spline-based functions. They therefore ideally combine with the paradigm of the Isogeometric Analysis (IGA), which applies the same spaces for description of geometry and Ansatz functions thus drastically reducing the effort for transition from CAD models to numerical analysis. Yet, in engineering practice, many more types of geometric models are used. These include Constructive Solid Geometry (CSG), which is frequently extended to parametric and feature-based design. Volumetric CAD models are also often described by indirect methods like the Boundary Representation (B-Rep). Completely different model types result from tomographic methods, where a body is defined only by a discretized density distribution.

In this paper, it will be shown how immersed boundary or embedded domain methods strongly support geometry-analysis integration in particular for solid structures. We will concentrate on the Finite Cell Method (FCM), which can use low- and high-order finite element spaces as well as spline-based, 'IGA-like' approximation spaces. For simplicity of description, we concentrate on linear elastic models, yet point out, that FCM has successfully been applied to a large variety of other problems like elasto-plasticity, contact problems, delamination, multi-physics and multi-scale problems.

The Finite Cell Method

Immersed boundary methods have been investigated in many variants (e.g. fictitious/embedded domain methods) since the 60ies of the last century [1]. Neittaanmäki and Tiba [2], Peskin [3], Del Pino and Pironneau [4], Mittal and Iaccarino [5], Glowinski and Kuznetsov [6] have made important contributions. More recent work refers to the CutFEM approach [7,8]. We consider in this paper the Finite Cell Method [9-11].

The basic idea of the Finite Cell Method can readily be explained with *Figure 1*, where it is formulated for the problem of linear elasticity. A bilinear form $a(\boldsymbol{u},\boldsymbol{v})$ representing the strain energy functional for a displacement field $\boldsymbol{u}$ and virtual displacements $\boldsymbol{v}$ is extended from its original domain of definition Ω to an extended domain Ω_e. $\boldsymbol{u}$ and $\boldsymbol{v}$ are from an appropriate trial and test space V. ε denotes the strain tensor and C the elasticity tensor. A volume load $\boldsymbol{f}$ and a surface traction $\boldsymbol{t}$ result in a load functional $F(\boldsymbol{v})$. The original weak

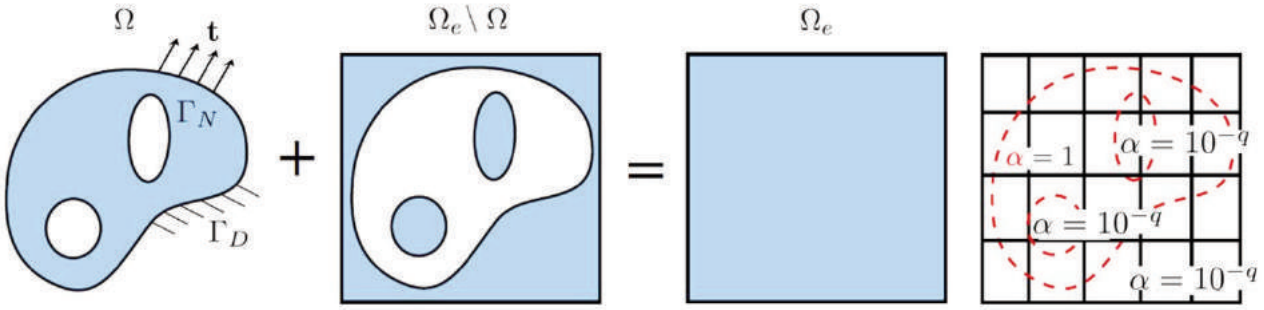


Figure 1: *The Finite Cell Method*

$$\text{Find } \boldsymbol{u} \in V \text{ such that}$$
$$a(\boldsymbol{u},\boldsymbol{v}) = F(\boldsymbol{v}) \qquad \forall \boldsymbol{v} \in V$$

$$a(\boldsymbol{u},\boldsymbol{v}) = \int_{\Omega_e} \boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{\alpha}(\boldsymbol{x})\boldsymbol{C} : \boldsymbol{\varepsilon}(\boldsymbol{u})\, d\Omega$$

$$F(\boldsymbol{v}) = \int_{\Omega_e} \boldsymbol{v}\cdot\boldsymbol{f}\, d\Omega + \int_{\Gamma_N} \boldsymbol{v}\cdot\boldsymbol{t}\, d\Gamma$$

$$\alpha(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \Omega \\ 10^{-q} & \text{if } \boldsymbol{x} \in \Omega_e \setminus \Omega \end{cases}$$

form of the elasticity problem is approximated by multiplying the elasticity tensor C by a function α, which is 1 in the original domain and obtains a very small value (typically 10^{-6} to 10^{-12}) in the fictitious domain $\Omega_e \setminus \Omega$. The rightmost part in *Figure 1* shows a background grid of 'finite cells' defined on the extended domain Ω_e. In principle, on this grid a classical numerical discretization can be applied. Low- or high-order finite elements can be used, or also knot span elements as defined in IGA are applicable. Using this grid of cells, the problem of mesh generation is completely avoided. In contrast to the existence of a finite element mesh only the knowledge of the membership of an integration point in a finite cell to either the interior or the exterior of the domain Ω is necessary.

The effort for transition from a geometric model to numerical analysis is thus drastically reduced, yet several new problems have to be solved. Among these are:

- ⇨How can boundary conditions in cells cut by the boundary of Ω be applied?
- ⇨In cut cells the integrand of the stiffness matrix is discontinuous. How can these integrals be computed precisely and efficiently?
- ⇨How can stability issues related to conditioning of resulting equation systems for the reformulated problem be handled?
- ⇨In numerical integration formulae for these cut cells, how can one decide quickly if an integration point is inside or outside of the domain?
- ⇨How can this Point-Membership-Test (PMT) be related to different geometrical models of the domain of computation?

Some central questions

In the following, we will briefly discuss the first three listed items and refer to related literature, whereas we discuss questions concerning point membership tests and show applications for different geometric models at the end of this short paper.

Boundary conditions: Neumann boundary conditions can easily be represented due to their integral nature in the weak formulation. The surface traction multiplied by the corresponding element shape functions have to be integrated over that part of the loaded surface, which is cut by the respective cell. In case of homogeneous b.c. nothing has to be done, as the surface integral is zero [10]. The case of Dirichlet boundary conditions is more complex. These b.c. also need to be applied in a weak sense. Various methods are available, like e.g. Nitsche's method [12-14].

Integration of cut cells: Numerical integration of cut cells is crucial for the accuracy and efficiency of the Finite Cell Method. For a survey with a comparison of different approaches, we refer to [15]. Here we concentrate on the simple, yet very robust version, the use of a cell-wise defined integration space-tree, which is successively refined towards the boundary of the domain of computation. The cell to be integrated is recursively bisected towards the location of the boundary. Thus, more and more of the generated sub-cells are either fully in or fully out of the domain and can be accurately integrated by Gaussian formulae. Only the smaller and smaller strip of cut sub-cells is affected by the discontinuity of the integrand.

Stability and conditioning of system matrices: Applying an indicator function α which is exactly zero outside Ω causes stability problems, in particular for cells with a very small material fraction. In these cases, techniques like the ghost penalty stabilization [12] can be applied. An alternative is to use a small but finite *α*. From a mechanical point of view, this is equivalent to embed the original structure in a 'soft' material. Thus the extended problem remains stable from a mathematical point of view, but the model itself is changed, introducing a modelling error and resulting in a slightly different 'exact' solution compared to the original formulation. Yet in practice, this modelling error is small enough (it is in the order of the strain energy in the 'soft', extended material!) so that it has no influence on an engineering relevant accuracy. For a mathematical analysis of the relation of modelling and approximation error, it is referred to [16]. Conditioning of the system matrix, which may also deteriorate in case of small cuts, can be controlled by the above-mentioned ghost penalty method, or in cases of non-vanishing *α* by Jacobi preconditioning and local orthogonalization [17]. In more complex cases like FCM combined with local hierarchical refinement, Additive-Schwartz-type preconditioning has been shown to be very successful [18,19].

Applications

Constructive Solid Geometry (CSG-models): CSG is a widely used modelling technique where a body is defined by a tree of geometric Boolean operations (union, intersection, difference) operating on primitives, which are in the simplest case mapped spheres, cylinders, cubes, tori etc. The library of primitives can be extended by more complex basic objects obtained e.g. by sweeps and lofts (see, e.g. [20]). The Point-Membership-Test can be

" labour-intensive pre-processing of problems with complex geometry can be simplified."

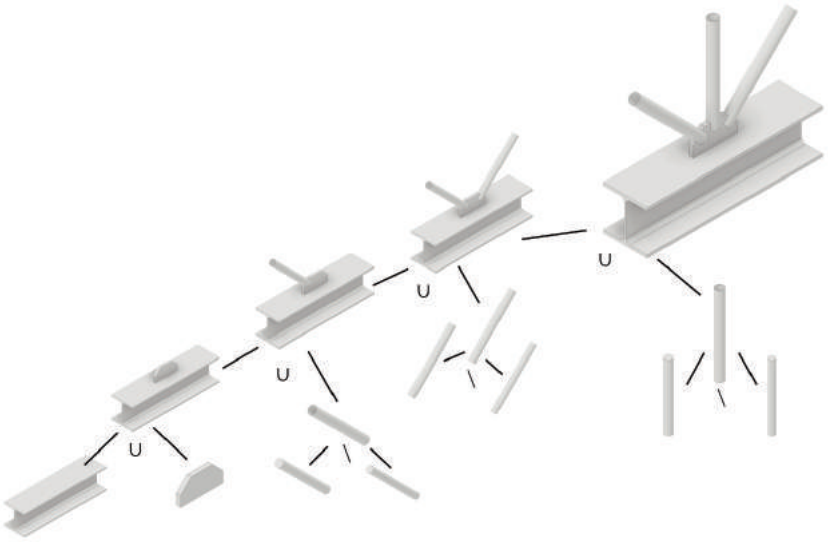


Figure 2: *Constrution tree for a steel joint*

carried out easily and efficiently. The geometric tree is equivalent to a tree of logic operations, and the elementary PMT operations are carried out on the primitives, where they are simple to perform. CSG-models can be extended to Parametric or Feature Based Geometric Models [21] by programming languages to define, constrain and interrelate geometric and topologic parameters. An example for a pipe built up as a CSG model is shown in *Figure 2*.

Figure 3(a): *Steel joint with finite cell mesh*

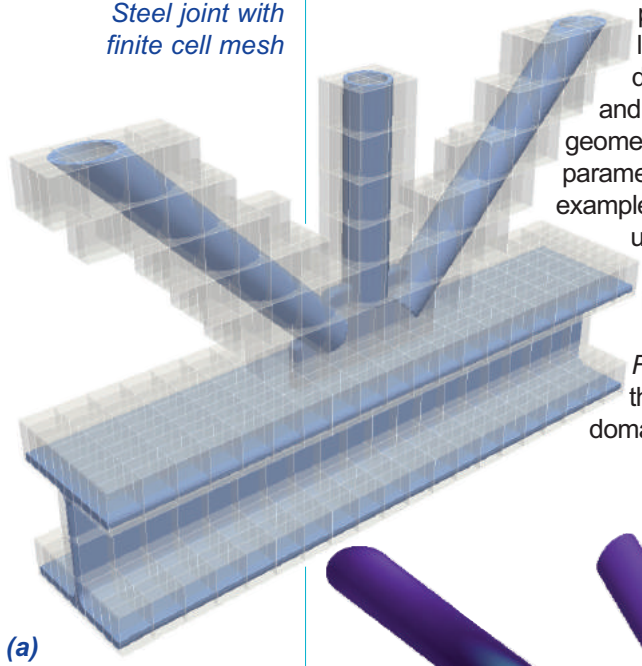
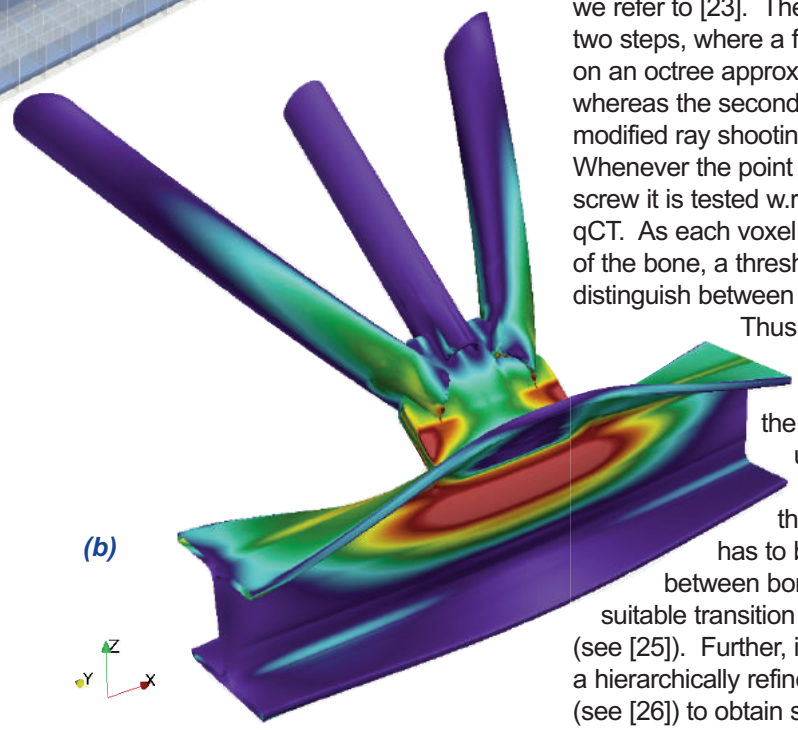


Figure 3a shows the embedding domain for a FCM computation (to be precise, only those finite cells which have a non-empty intersection with the pipe!) and *Figure 3b* the von Mises stress on the deformed structure. The major advantage of FCM compared to a finite element computation becomes obvious in *Figure 4*. Here, not only some geometric parameters have been changed, also the number of holes in the attachment plate is different from the example in *Figure 3*. Any finite element analysis would need the generation of a new mesh, whereas no regeneration is necessary for FCM. The new structure is identified on the level of the Point-Membership-Test for the integration points of the cell matrices.

(a)



(b)

Figure 3(b): *Steel joint with equivalent stress*

Mixed Voxel-based and B-Rep Models:
In this final example, we will demonstrate the possibility to use different geometric descriptions in one joint geometric model. *Figure 5* shows a sectional cut through a quantitative computer tomogram (qCT) of a human vertebra together with a fixation screw implanted in the bone. The qCT stores in a voxel structure Hounsfield values of the bone, which are the basis for computation of the local elasticity modulus (see, e.g. [22]). The screw is modelled by its boundary representation (B-Rep), where the surface is first defined by NURBS and then discretized into a facetted model. The PMT for this combined model is now performed as follows: For an integration point of the finite cell computation a first (Boolean) test is performed, deciding if it is inside the screw. For efficient methods to perform this test even in cases of 'dirty' B-Rep models, i.e. those which have small gaps or overlaps, we refer to [23]. The test is performed in two steps, where a first, coarse step relies on an octree approximation of the structure, whereas the second, fine grain step uses a modified ray shooting technique (see [24]). Whenever the point of interest is outside the screw it is tested w.r.t. the voxel model of the qCT. As each voxel represents the density of the bone, a threshold value is defined to distinguish between bone and empty space. Thus, this model can be interpreted as a level set description, where the critical value is not (as usual) zero, but the predefined density threshold. Special care has to be taken on the interface between bone and screw, where suitable transition conditions are defined (see [25]). Further, in this example we use a hierarchically refined grid of finite cells (see [26]) to obtain sufficient efficiency and

accuracy despite the highly complex geometry of this example. *Figures 6a and 6b* show equivalent strains in sections of the structure.

Conclusions

We have presented the Finite Cell Method, which is a fictitious domain approach that allows for low-, high-order as well as 'IGA-like' approximation spaces. Thanks to its versatility, the FCM can be easily combined with different geometric models supporting a seamless discretization process. In this way the labour-intensive pre-processing of problems with complex geometry can be simplified. Since the FCM inherits most of the properties of finite elements and IGA, it represents an attractive simulation approach that is applicable to challenging problems of Computational Mechanics. ●

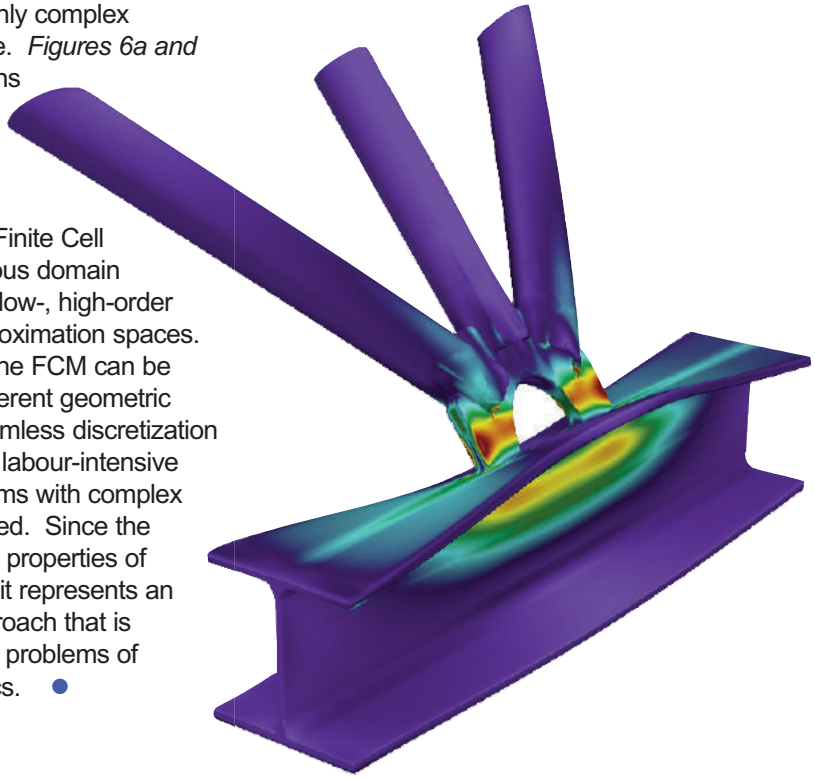


Figure 4:
Equivalent stress on modified structure

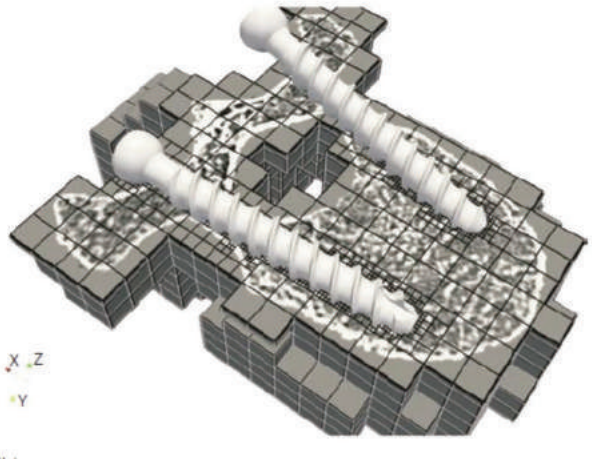
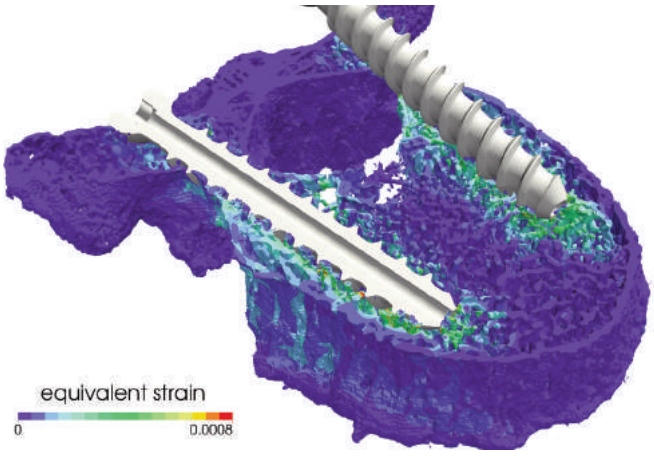


Figure 5:
(a) *qCT scan of a human vertebra*

(b) *BRep-Model of screws embedded in hierarchically refined FCM grid*



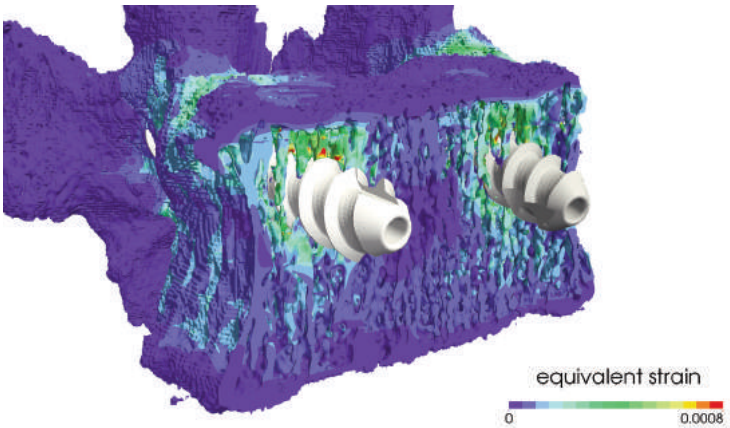


Figure 6 (a) and (b):
Equivalent strain on two sections

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Geometrically-Compatible Dislocation Patterns and Multiscale Dislocation Pattern Dynamics

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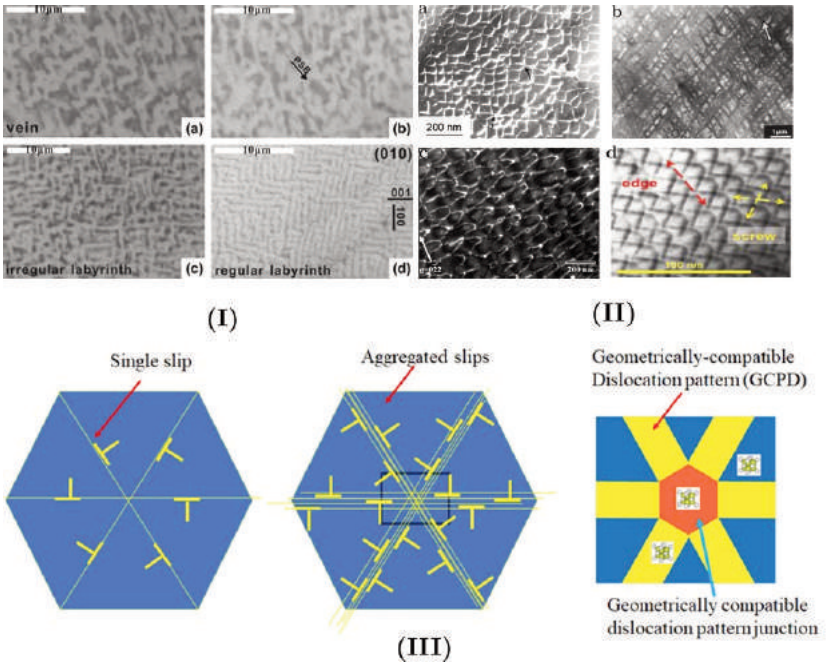
Dislocations in a deformed crystal tend to aggregate into various dense formations separated by relatively dislocation free regions. These dense formations are called dislocation patterns that underlie most important crystal plasticity features such as work hardening and strain localization. Depending on slip geometry, external loading and temperature, rather different pattern morphologies emerge e.g. labyrinth, ladder, wall, and cell structures) emerge from deformed crystals as shown in *Figure 1*.

Understanding spontaneous emergence of dislocation patterns during plastic deformation has been an outstanding and critical task in developing a physical mechanism-based crystal plasticity.

Figure 1:
(I) Dislocation pattern formations under cyclic loading in a Silver single crystal observed from different lattice orientation (From Li et al.(2009) [8]), and
(II) Dislocation pattern formations under cyclic loading in a Nickel single crystal observed from different lattice orientation (From Bugue et al. (2001) [9]), and
(III) Concept of geometrically-compatible dislocation patterns



During the past decades several phenomenological continuum models of dislocation pattern were proposed e.g. Kubin and Canova [1], Kratochvil and Saxlova [2], Aifantis [3], and more recently, Hochrainer et al. [4, 5, 6], and Groma et al. [7], but none of them were developed or derived based on atomistic considerations through a systematic and controlled coarse-grain procedure, and none of them has lead to an valid crystal plasticity theory yet.

Two bottom-up approaches towards "first-principle" based crystal plasticity are: molecular dynamics and discrete dislocation dynamics, which have received much attentions in recent years. Atomistic-based molecular dynamics has been extensively used to study some of the isolated interaction mechanisms, but it is limited by the spatial and temporal resolution that the current computational technology has diculties to resolve. In particular, because of such limitation, the molecular dynamics approach has diculty to properly capture the long-range character of dislocation stress field, heat dissipation mechanism, and obviously, the statistical nature of crystal plasticity. Alternatively, discrete Dislocation Dynamics (DD) is another extensively-used approach that attempts to delineate the overall motions or effects of large scale dislocation ensembles at mesoscale by decomposing dislocation lines of arbitrary curvature into piecewise segments based on linear elasticity theory. In addition to some other limitations, DD is also limited by its computational capacities failing to capture the microstructure of aggregated dislocations, or more specifically, the dislocation patterns, so that we cannot study long range flow stress effects based on dislocation motions and hence crystal plasticity itself.

Figure 1 (I) and (II) display the dislocation pattern formations for various crystals. They showed that for a given crystal and along given crystallographic directions the dislocation pattern may be related to the original crystal lattice structure or microstructure. Thus, just like geometrically necessary dislocations, we hypothesize that there exist a class of *geometrically*

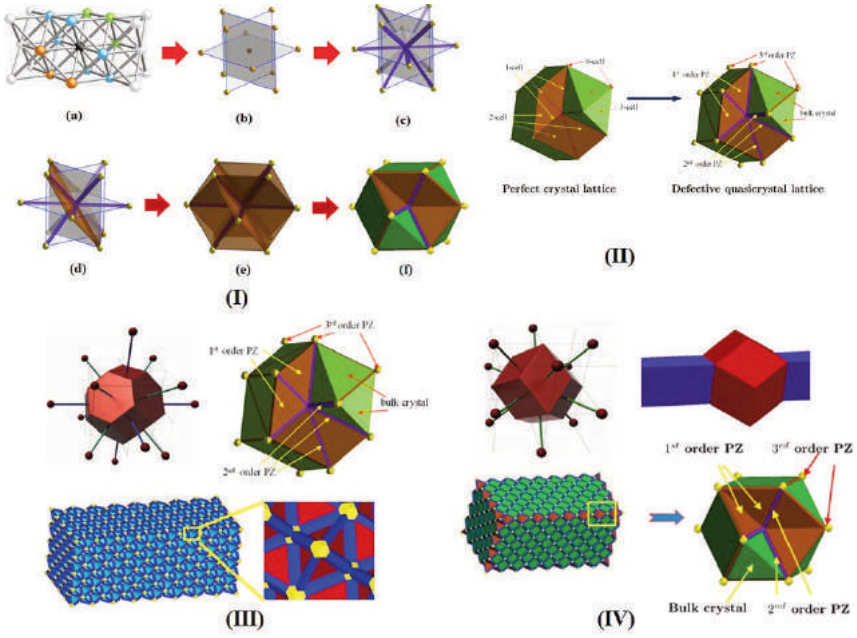


Figure 2:
(I) How to form geometrically-compatible dislotion pattern (GNDP) formations lattice;
(II) How does a lattice simplex become lattice CW complex;
(III) BCC geometrically-compatible dislocation patterns, and (III) FCC geometrically-compatible dislocation patterns

compatible dislocation patterns. Such geometrically-compatible dislocation patterns are aggregated dislocation pattern growing out of particular individual atomic sites and atomic planes forming a geometrically compatible network that is a natural extension of the original crystal microstructure.

Based on the evidences obtained from MD simulations *(see Figure 3 (II))* in the multiscale crystal defect dynamics, we postulate that the geometrically-compatible dislocation pattern in crystal are related to the dual super-lattice of the original crystal lattice in the early stage, and the actual dislocation patterns may emerge from the dual super lattice mesh, depending on loading condition and loading history.

Starting 2014, in a series of works [10, 11, 12], we have discovered the geometrically-compatible dislocation patterns in both BCC and FCC crystals, and we have since developed a Multiscale Crystal Defect Dynamics (MCDD), which is a geometrically-necessary or geometrically-compatible dislocation pattern dynamics.

Figure 1 (III) show how a geometrically-compatible or geometrically-compatible dislocation pattern is formed. In *Figure 2*, we show the geometrically-compatible dislocation pattern formations in both BCC *(Figure 2 (III))* and FCC *(Figure (IV))* crystals.
To simulate the actual geometrically-compatible dislocation pattern formations, we create a so-called pre-dislocation pattern finite element mesh in the domain of interests, this special dislocation pattern-like FEM mesh is a global cover or partition of crystal lattice space that is topologically the same as that of the geometrically-compatible dislocation pattern.

In some cases, this pre-dislocation pattern mesh is in fact a quasi-lattice structure that is resulted from the symmetry broken of the original lattice structure. This long-range order geometrically-compatible dislocation pattern partition of the original lattice space is part of a “heritage” of the crystal microstructure. Based on this development, we postulate that for a given type of crystals, it is only prone to certain types of defects or damage that are associated with the geometrically-compatible pattern of the original lattice space.

In *Figure 3 (I)*, we compare the dislocation pattern observed in experiments with that constructed in MCDD finite element mesh. One can see that the resemblance between the two.

Towards an atomistic-informed crystal plasticity

Based on the concept of geometrically-compatible dislocation pattern, we have developed a multuscale crystal defect dynamics (MCCD) (see [10, 11, 12].
The basic idea of MCDD method is to embed the long-range order pre-defect process zone or the geometrically-compatible dislocation patterns a priori as the lattice finite element mesh, and then let crystal material evolving itself under external loads to select its own failure pathes or ramifications based on the finite numbers of combinations of possible dislocation patterns that have been embedded into the MCCD finite element mesh according to an atomistically-informed constitutive equation without solving any ad hoc defect pattern evolution equations.

According to the invariant properties of dislocation dynamics, these three-dimensional dislocation may be scalable, and it may be consisted of different “order ” of process zones that are lacing together many bulk crystal elements, which have low dislocation density (dislocation cells). In the modeling, Different dislocation pat-

terns are being modeled as the combinations of **different order of process zones**:
(1) Dislocation cell or sub-grain mainly consists of bulk crystal elements;
(2) Dislocation wall is formed by thin layer process zone elements;
(3) Dislocation labyrinth or network is formed by thin prism-shaped process zone,
and (4) Volume defect is formed by void-shaped process zone element, which may serve as the model for dislocation pattern junctions. They may be the sites for precipitates,dispersants, inclusions, or voids.

Based on the hypothesis that the dislocation pattern at the early stage geometrically or topologically resembles the pre-dislocation process zone mesh discussed above, or they are a subset of the pre-dislocation process zone finite element mesh, by simulating the dynamics of the process zone evolution, we may be able to trace and monitor the time evolution of dislocation patterns, and hence the plasticity of the crystal. Based on this assumption, we impose additional kinematic constraints on the pre-dislocation process zone elements: The deformation inside every bulk element is uniform or homogeneous, whereas all the process zone elements will undergo inhomogeneous deformations, because part of them are dislocation patterns. In order to capture dislocation patterns we employ higher order Cauchy-Born rule based strain gradient theory. These kinematic conditions are reflected by the FEM interpolation functions used in different order of process zone elements. In computations, we add different bubble models in the higher order process zone elements (See: Fan and Li [15], Lyu et al.[16]), Urata and Li [17]) to provide a high order displacement field.

As discussed above, the formation of dislocation patterns significantly relies on the active slip systems [13]. *Figure 4 (b) and (c)* show dislocation pattern formations or dislocation cell structures, during cyclic loading for FCC crystal (Copper and Nickel) in different orientations in the stereographic triangle, which is compared with the stereographic projections of MCDD pre-dislocation pattern mesh in the same orientation *Figure 4 (b) and (c)* .

By comparison of *Figure 4 (b) and (c)*, one may find that the experimental observations of dislocation pattern formations agree with that of MCDD

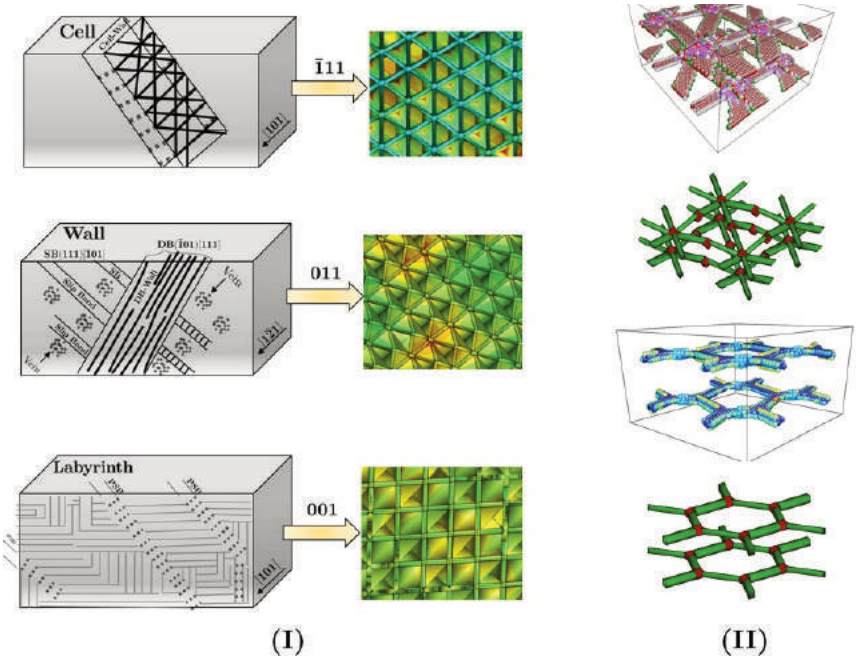


Figure 3:
(I) Comparison of substructure or formations of dislocation patterns observed in fatigue experiments [13] and that obtained in MCDD simulations in different orientations;
(II) Dislocation patterns in FCC crystal Cu and in BCC crystal obtained in MD simulations compared with the corresponding mesh of MCDD pre-dislocation meshes

pre-dislocation mesh patterns in respective orientations, which suggests that at least the mechanism of the early dislocation pattern formation is not a random or stability event, but rather a lattice geometric configuration related event that is completely determined by the crystalline

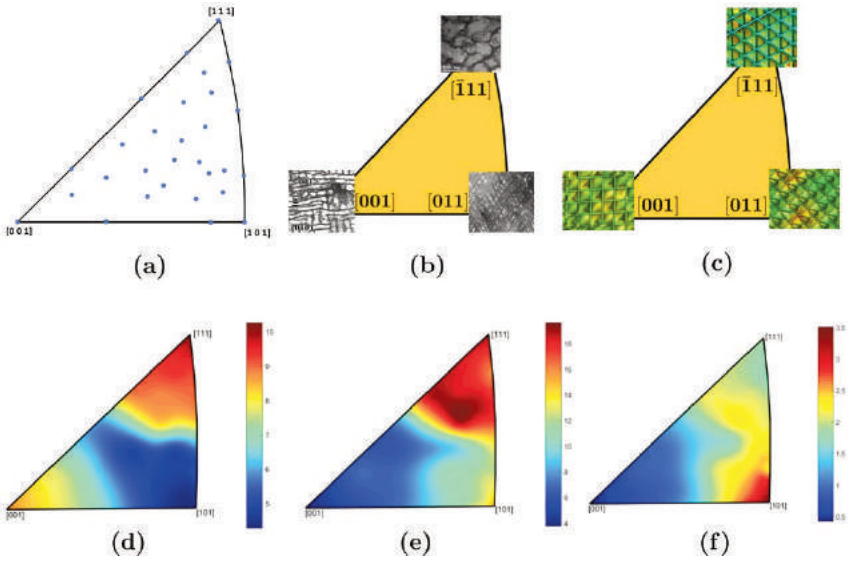


Figure 4:
(a) Stereographic triangle showing the 29 crystallographic orientations; (b) (c) Comparison of dislocation pattern formations and substructures in different orientations with experiments [9, 14], and (d), (e), (f), contour plots of tensile and compressive yield stress and the ratio of compressive stress and tensile yield stresses in different orientations [12]

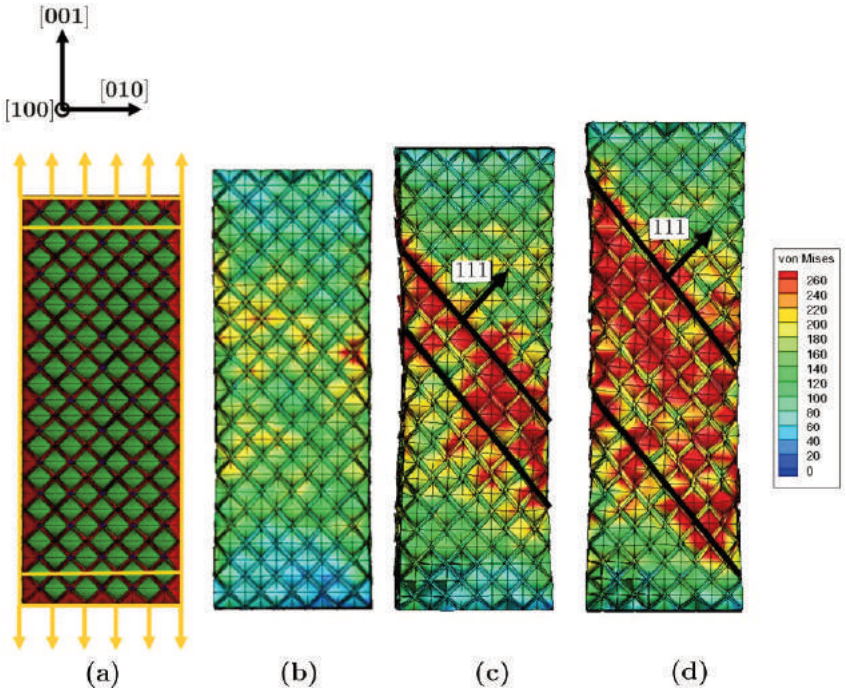
" multiscale crystal defect dynamics ... links atomistic information with long-range order dislocation pattern dynamics, ... it allows us to establish an atomistically-informed crystal plasticity theory based on dislocation pattern dynamics.."

materials' microstructure. In addition, *Figure 4 (b) and (c)* show three types of dislocation patterns of dislocation cell structures observed in experiments, which are compared with the MCDD mesh structure in the same orientation. Again, we can see that the remarkable resemblance between the two in each every orientations.

To demonstrate MCDD is an atomistically-informed crystal plasticity theory. We employed MCDD to simulate anisotropic plasticity at grain scale and to study the influence of crystal orientation on dislocation nucleation and slip system activation.

Crystal plasticity is an anisotropic inelastic deformation theory. During mechanical loading, crystalline material responses or behaviors depend on both crystal microstructure as well as the external load orientations. In the classical Taylor crystal plasticity, dislocation motion in single crystals is thought to be governed by the critical resolved shear stress (CRSS) via Schmids law [18]. However, Taylor crystal plasticity theory may still be considered as a phenomenological theory, because the value of CRSS is either given on an empirical value, or taken from the fine scale first principle simulation, and it is not within a self-consistent framework of crystal plasticity itself. Moreover, the classical plasticity may not be able to capture some fundamental aspects of the physical phenomenon, i.e. the non-Schimid stress. To simulate the local plastic deformation, we employed MCDD to simulate formulation of shear band. A copper specimen with size *16nm x 16nm x 40nm* is investigated. A constant velocity (corresponding to a strain rate on the order of 10^{10}/s is applied at the top and bottom boundary along the [001] direction as shown in *Figure 5(a)*. In *Figure 5 (b), (c), and (d)*, we display the formulation of shear band in (111) plane, which is the corresponding slip plane for FCC crystal. This example shows that MCDD has the ability to simulate dislocation nucleation and shear band formulation.

Figure 5:
(a) MCDD pre-dislocation mesh, and formulation of shear band in (111) plane with strain (b) 2% (c)15% and (d) 15% and (d)25%.



Discussions

The main novelty of the multiscale crystal defect dynamics is that it directly links atomistic information with long-range order dislocation pattern dynamics, so that it allows us to establish an atomistically-informed crystal plasticity theory based on dislocation pattern dynamics. The main developments of the multiscale dislocation pattern dynamics based crystal plasticity approach are:

1. Work hardening during plastic deformation of a crystal is associated with significant changes in dislocation microstructure. The increase in dislocation density on the specimen is accompanied by the spontaneous emergence of regions of low dislocation density and clusters of high dislocation density which to a large extent persist upon unloading. These metastable structures are denoted as dislocation patterns. The fundamental hypothesis of MCDD is that these dislocation microstructure depend on the original crystal microstructure, and one may identify possible defect pattern regions by geometrical analysis of the original crystal lattice;
2. The mathematical foundation of MCCD is based algebraic topology and exterior differential calculus. The rigorous mathematical and physics foundation of MCDD renders it a precise quantitative scientific method or approach;
3. MCDD can relate the size-dependent plastic deformation to fundamental physics of defects, i.e. nucleation, multiplication, annihilation, interactions and transport of dislocations and

vacancies;
4. It is an atomistically-determined formulation while preserving the continuum character. MCDD model transcends length scale directly from nano meter scale to millimeter scale, which does not need any hierarchical modeling and computations;
5. As an atomistic-informed continuum formulation, MCDD preserves the well-posed mathematical structure of continuum physics by describing the problem as a rigorous initial-boundary value problem in terms of partial differential equations. Moreover, the MCDD multiscale formulation minimizes ad-hoc assumptions and free parameters (as used extensively in strain-gradient and other scale-dependent plasticity theories;
6. It provides a faster computational framework, and hence it has more feasible and applicable to macroscale objects than molecular dynamics, and probably even than discrete dislocation dynamics, and
7. The spontaneous emergence of heterogeneous dislocation patterns is a conspicuous feature of plastic deformation and strain hardening of crystalline solids. Currently, almost all dislocation pattern theories are empirical continuum theory. The proposed multiscale crystal defect dynamics theory is derived based on atomistic molecular dynamics through systematic coarse graining procedures, and hence its physical modeling fidelity is significantly improved over other dislocation pattern models as well as discrete dislocation dynamics, while retaining almost the same or even less computation cost. To the authors' best knowledge, MCDD may be the first atomistically-informed dislocation pattern dynamics in the literature. ●

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Practical 3D-Engineering Fracture Mechanics Analysis

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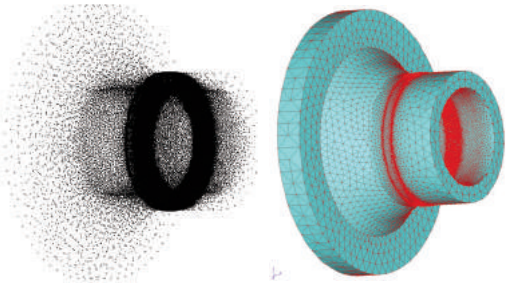
In the present article, the author would like to present 3D-practical engineering fracture mechanics analyses. Many engineers and researchers may believe that meshing is a major obstacle in 3D-fracture mechanics analyses based on the finite element method. Generating a 3D-finite element model for an engineering structure is not a trivial task, even today. However, finite element models are created daily from CAD data in the design processes of engineering products, assisted by automatic mesh generation software. Engineers then perform finite element analyses to evaluate their designs.

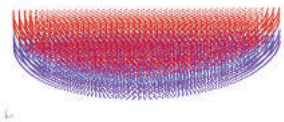
When cracks exist in a 3D-structure, there is a tendency to think that the meshing is troublesome. The reason for this is that a mesh with regularly arranged hexahedral finite elements is generally required in the vicinity of the crack front. This is a strong constraint in generating a finite element model. When we generate a 3D-finite element model for a structure using an automatic meshing program, we generally adopt tetrahedral finite elements. In other words, the use of tetrahedral finite elements is required when an automatic meshing scheme is used. Since crack analyses generally require the use of hexahedral finite elements, manual operations by the analyst are necessary in order to generate a finite element model for fracture mechanics analysis. In order to avoid meshing, the eXtended finite element method (X-FEM) and generalized finite element method (G-FEM) were proposed. These methods became popular approaches to crack analysis [1, 2]. These methods have increased in popularity. On the other hand, approaches based on the ordinary finite element method have been proposed [3, 4]. These approaches require special care in their finite element discretizations in the vicinity of the crack front such that regularly arranged hexahedral elements must be placed. These are popular approaches. In this article, a somewhat simpler method by which to deal with three-dimensional crack problems is introduced. Tetrahedral finite elements are used even in the immediate vicinity of the crack front.

Research and development on a meshing strategy has been carried out by Kawai et al. [5] for structures with cracks. The finite element mesh consists of only tetrahedral finite elements. We refer to this approach as a point-based method. A group of points representing the solid as a whole and a surface patch are first supplied by the analyst, as shown in *Figure 1(a)*. The convex nodes and the surface patch are extracted from a finite element mesh without any cracks. In this process, a commercial finite element mesh generation program may be used. Then, an analysis must supply a group of points representing a crack and its vicinity, as shown in *Figure 1(b)*. A small in-house program was written for the present study. Hence, the group of points for the crack and its vicinity are inserted among the points for the whole structure. A constrained Delaunay tessellation technique is then applied to generate the mesh consisting of the tetrahedral elements, as depicted in *Figure 1(c)*. The constrained Delaunay tessellation technique avoids the generation of tetrahedrons that span both sides of the crack face. Multiple crack problems, as shown in *Figure 2*, can also be modeled without much difficulty. The distributions of the mixed mode stress intensity factors were computed by the virtual crack closure-integral method (VCCM) [6] without any

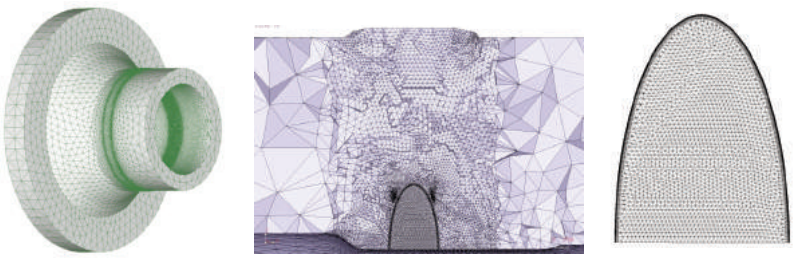
Figure 1:
Example of finite element mesh generation. Group of points and a surface patch provided by the analyst and the generated finite element mesh. This is an example for a reactor pressurizer surge nozzle



(a) A group of points and surface patch for the whole structure



(b) A group of points for crack



(c) Finite element mesh (left: whole view, center: section with a crack and right: crack face)

Figure 2:
Example of multiple crack analysis (finite element model, stress distribution, and the results of the SIF computations)

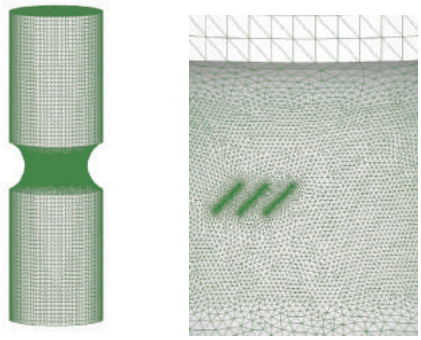
difficulty. The results are also shown in *Figure 2*. The finite element mesh for the three-crack problem was created by TSV-Crack [7], in which the crack mesh option was developed following the success of the VCCM for quadratic tetrahedral finite elements [6].

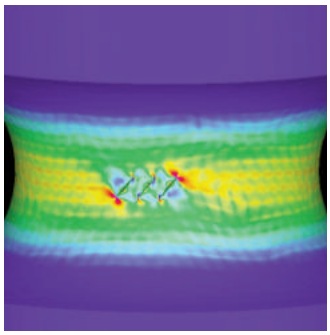
Brief descriptions of methodologies for computing the crack parameters and example problems

Researchers and engineers may have believed that hexahedral finite elements must be placed in the vicinity of the crack front due to methodologies for evaluating crack parameters, such as stress intensity factors, the energy release rate, and the J-integral. Method for computing the crack parameters include the VCCM, the virtual crack closure technique (VCCT), the domain integral (DI), and the equivalent domain integral (EDI) method for the J-integral and the interaction integral method. When the integral domain is set for the EDI, we tend to assume that the domain must have a smooth outer shape. For example, a cylindrical shape is often assumed. Then, hexahedral finite elements must be arranged so that the integral domain can be set in a layer-by-layer manner. Hence, the integral domain has a smooth shape.

However, as described in Okada and Ohata [8] and Dimon and Okada [9], the smoothness of the outer shape of the integral domain and the use of regularly arranged hexahedral finite elements in the vicinity of the crack front are not essential requirements in the domain integral method. The essential requirement is that the virtual crack extension vector, which is interpolated in the integral domain, must be continuous and piecewise differentiable. There is no essential requirement on the outer shape or the arrangement of the finite element mesh.

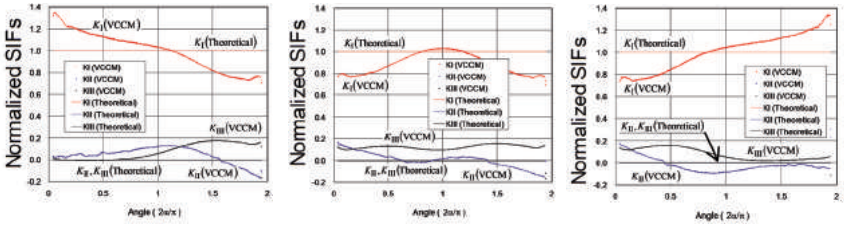
Examples are shown in *Figures 3 and 4*. *Figure 3* shows an example of an integral domain that has an angular outer shape, and *Figure 4* shows an example of stress intensity factor evaluation under a mixed mode load using an unstructured mesh,





(b) Distribution of the von-Mises stress in the vicinity of the cracks. The color indicates the magnitude of the stress. Red is high and blue is low

(a) Finite element mesh consisting of the quadratic tetrahedral elements (top left: whole specimen, top right: magnified view of the crack mouths and below: crack face). The round bar specimen is subject to a torsional torque



(c) The results of the computations of the stress intensity factors for the inclined three cracks (left, center and right). "Theoretical" indicates the theoretical solutions for the embedded circular crack in an infinite elastic body under the respective tensile remote stress

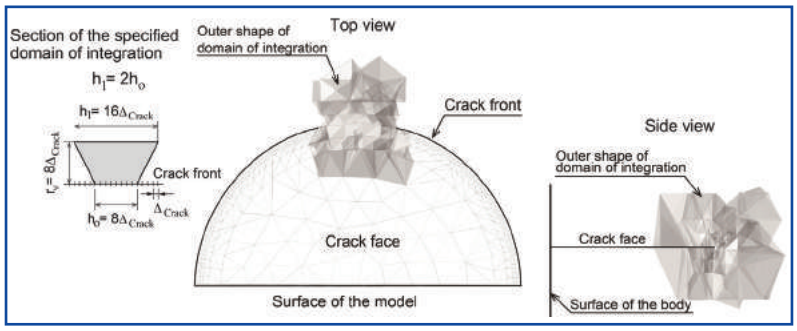
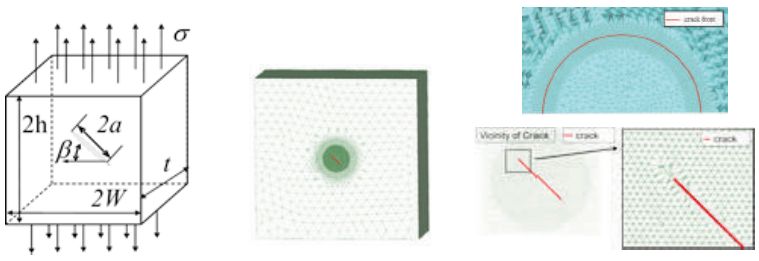
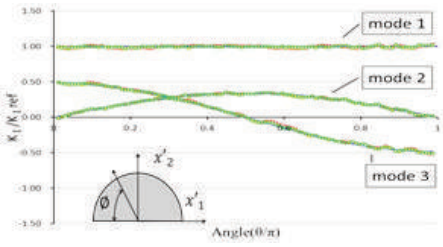


Figure 3:
Example of an angular integral domain for the J-integral and interaction integral

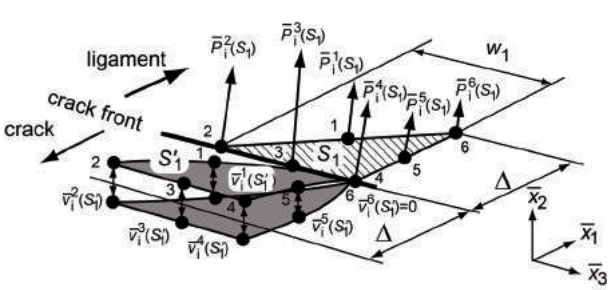


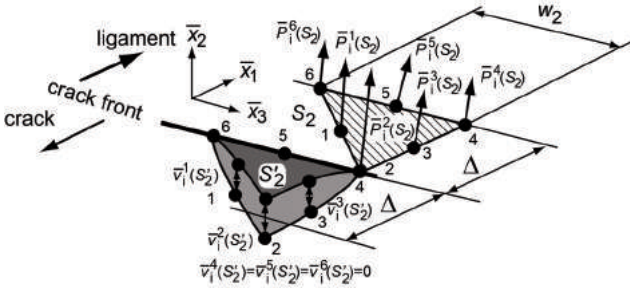
(a) Inclined embedded penny shaped crack in an infinite elastic body subject to the remote tension and its finite element mesh. (left: the infinite elastic body with the embedded inclined penny shaped crack, center: the whole view of finite element model, right: crack face and magnified view of the crack that is modeled only one layer of crack face element



(b) The distributions of the stress intensity factors that were computed by the interaction integral method. Three different sizes were set for the integral domain. They gave almost the same results

Figure 4:
Example of computations of the stress intensity factors using unstructured finite element mesh





$$G_I = \frac{K_I^2}{E'} \approx \frac{1}{S_2} \sum_I \bar{P}_{S_2}^I \times v_{S_2}^I$$

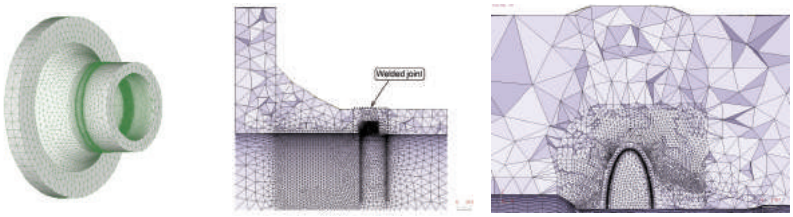
$$G_I = \frac{K_I^2}{E'} \approx \frac{1}{3S_1} \sum_I \bar{P}_{S_1}^I \times v_{S_1}^I$$

Figure 5: *Concept of the VCCM. The faces of finite elements are virtually closed by nodal forces. The energies required in order to virtually close the element faces are related to the energy release rate GI and the stress intensity factor KI. Here, the mode I problem is considered as an example*

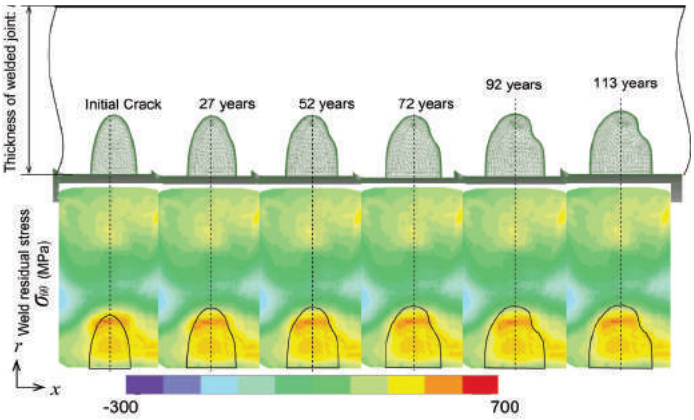
even in the vicinity of the crack front. Only one layer of discontinuity was inserted in the unstructured mesh.

On the other hand, crack propagation problems have also been solved (see Nose et al. [10]) using the VCCM [6] for the tetrahedral finite element. The VCCM computes the stress intensity factors based on energy change when the faces of finite elements adjacent to the crack front are virtually closed, as shown in *Figure 5*. In *Figure 6*, an example of a crack propagation problem of the pressurized surge nozzle for a nuclear pressure vessel is shown. Stress corrosion cracking (SCC) is assumed in welded joints between dissimilar materials. The growth of such cracks is driven by the weld residual stress. In this analysis, computationally predicted weld residual stresses were applied.

Figure 6: *Example of analysis of SCC propagation driven by the weld residual stress*



(a) The finite element mesh that was used to perform an analysis on SCC propagation driven by the weld residual stress (left: whole view, center: section of including the crack face and left: the magnified view of the initial crack)

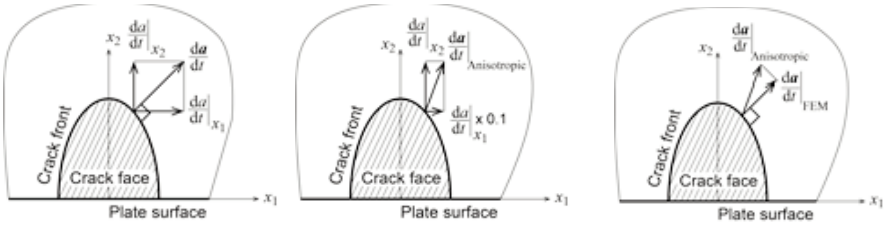


(b) The result of SCC propagation analysis. The shapes of crack after its propagation are superposed on the distribution of the weld residual stress

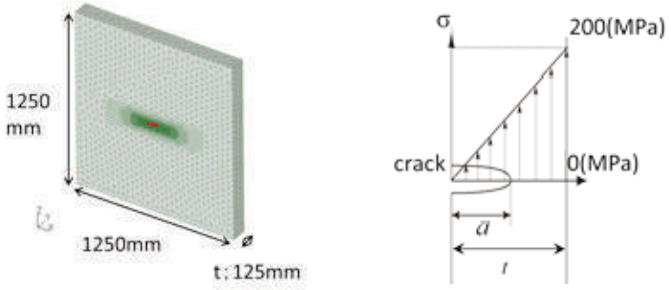
In the following, we apply hypotheses to the computational crack propagation simulations, as presented in Sugawara et al. [11]. During the welding processes, not only the weld residual stress but also material anisotropy is produced. We introduce a hypothesis on the crack propagation rate. The SCC (Stress Corrosion Cracking) propagation may have some directional preference as a result of the solidification rate of, for example, the weld metal and residual stresses. The material anisotropy can easily be assumed in the fatigue crack propagation law. An example is presented in *Figure 7(a)*. The vector representing the crack propagation rate is decomposed in the surface and depth directions and then reassembled using various weights. *Figure 7 (b)* shows the mesh and the variation of assumed stress in the thickness direction. *Figure 7(c)* shows that due to the increasing stress in the depth direction, the crack was found to take on a balloon-like shape when the anisotropic crack propagation law was not adopted. However, due to the influence of the anisotropic crack propagation law, the crack growth in the depth direction dominated that in the surface direction, as seen in *Figure 7 (d)*. The crack added its depth only.

The present technique was applied to a large-scale finite element fracture mechanics analysis, as seen in Arai et al. [12]. *Figure 8* shows the finite element analysis for a section of a nuclear pressure vessel. A crack was assumed to emanate and grow at the inner surface of the nozzle. The configurations of the section and the nozzle are presented in *Figure 8*. A finite element model for the section is presented. The model has approximately 72 million elements and 100 million nodes. An SCC propagation analysis under an applied internal pressure was then carried out. The crack grew as shown in *Figure 8*.

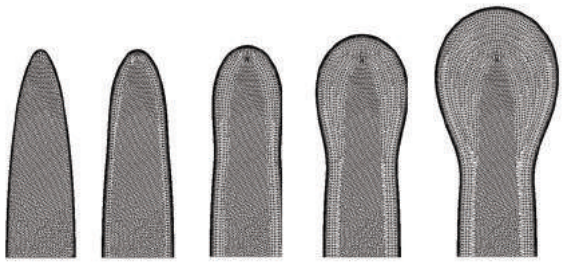
Figure 7:
Fatigue crack propagation under the anisotropic crack propagation law and increasing stress amplitude in the crack growth direction



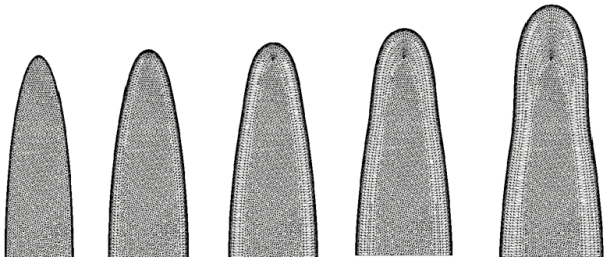
(a) Hypothesis on the crack propagation rate. Left: Crack propagation is assumed perpendicular to the crack front. center: The rate of crack propagation in the surface direction is set to be 1/10 of its original magnitude. The vector of crack propagation is assembled again. and right: The vector of crack propagation is projected to the normal direction of the crack front. Then, the crack propagation analysis is carried out



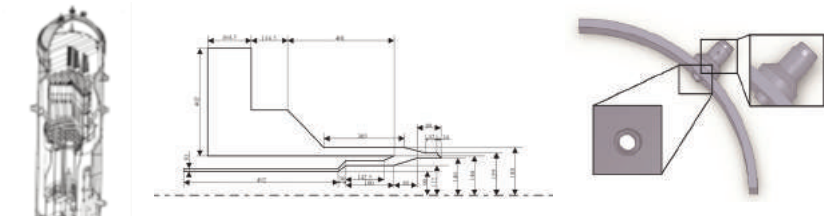
(b) Finite element mesh and the dimensions of the plate for which the crack is assumed (left) and the assumed amplitude of fatigue load (right)



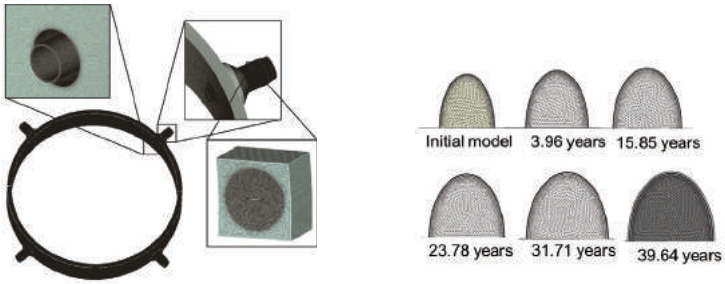
(c) The results of crack propagation analysis under the isotropic crack propagation law. The crack grew to be a balloon-like shape



(d) The results of crack propagation analysis under the hypothesis of anisotropic crack propagation law. The crack extends to the depth direction



(a) The configurations and the simplified CAD drawing of nuclear pressure vessel. Left: The general configuration of the nuclear pressure vessel [14]. Center: The section of nozzle part and Left: CAD drawing of a quarter section part containing the nozzle. A crack was assumed to exist the inner wall of the nozzle part



(b) The large scale finite element model containing more than 100 million nodes and the evolution of the crack face as the result of SCC propagation analysis. SCC was assumed to be driven by the applied internal pressure on the inner wall of the pressure vessel and the nozzle and on the crack faces

Development of the present software system

The crack and crack propagation software consist of a number of loosely coupled programs and shell scripts to perform mesh generation, FEA preprocess, FEA, and FEA postprocess, for example.
We refer to these analysis phases. The general flow chart of the analysis system is shown in *Figure 9*. There are a number of short programs and shell scripts to perform tasks in the analysis system. Therefore, they can be modified easily in the laboratory. Moreover, standardized data formats and structures, such as nodal coordinates, element connectivity, and boundary conditions, are used to describe data. Thus, programs to carry out certain analysis tasks, such as computing the stress intensity factors, can be changed. For example, the VCCM [6] and the interaction integral method of Daimon and Okada [9] can be used to compute the stress intensity factors. Programs for both of these methods use almost the same standardized input dataset. Therefore, they are exchangeable. In addition, such as the influence of the crack face load, options can be added to the programs by the analyst. The finite element programs are also exchangeable. The default option in our software system is Adventure Solid [13], which is open-source FEA software for large-scale computations. Using a small data translator, we may use commercial FEA software, such as MSC.Marc or NASTRAN.

Conclusion

In the present article, examples of fracture mechanics analyses using the ordinary finite element method were presented. The point-based mesh generation scheme was briefly introduced. This method can generate a mesh with cracks consisting of only tetrahedral finite elements. Such finite element meshes have been considered unsuitable for crack analysis. Hence, methodologies that can accurately compute stress intensity factors using meshes consisting of tetrahedral elements

Figure 8:
Example of large-scale crack propagation analysis

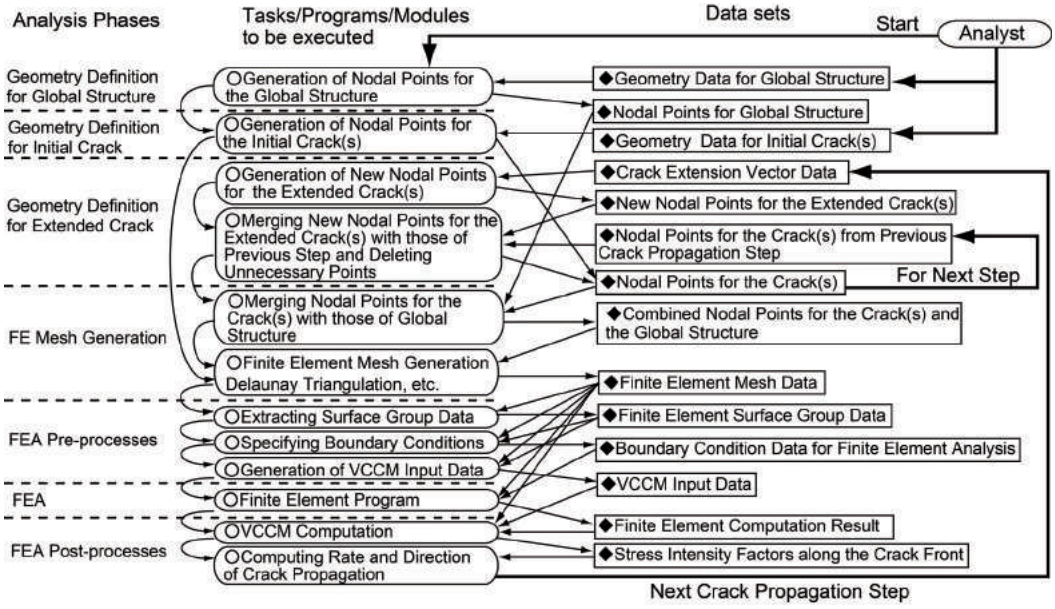


Figure 9: *General flow chart of the crack propagation analysis system*

only were developed and briefly discussed in the present article. Since certain methods allow us to use the unstructured mesh, even in the immediate vicinity of the crack front, such methods can be used to solve large-scale problems, as shown in the last example problem that was presented.

Finally, the software development strategy in our laboratory environment is briefly described. We are developing our methodologies under a software platform that loosely connects programs and shell scripts, including in-house programs/scripts and commercial/open software. Development continues in order to achieve more realistic fracture simulations that can be used for the analysis of structural integrity assessment of engineering structures. ●

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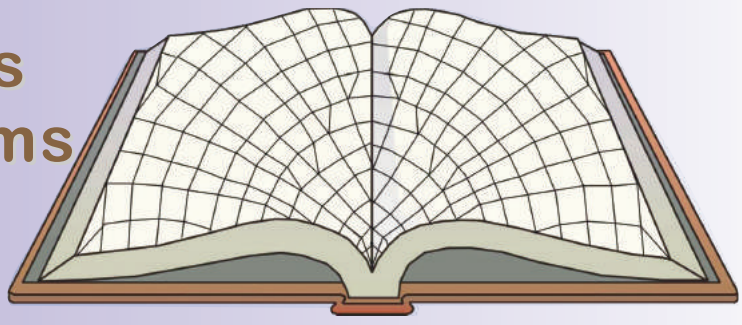
Numerical Methods for Inverse Problems



Michel Kern
ISTE & Wiley, London, UK and Hoboken, NJ, USA, 2016

BOOK REVIEW

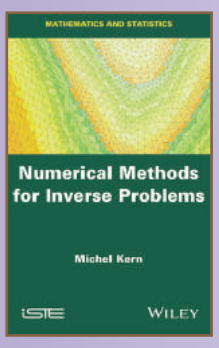
ISBN: *978-1-848-21818-5, 228 pages, hard cover, $115 (List Price).*
Contents: *Preface; 1: Overview of Inverse Problems; 2: Examples of Inverse Problems; 3: Integral Operators and Integral Equations; 4: Linear Least Squares Problems – Singular Value Decomposition; 5: Regularization of Linear Inverse Problems; 6: Nonlinear Inverse Problems – Generalities; 7: Some Parameter Estimation Examples; 8: Further Information; Appendix 1: Numerical Methods for Least Squares Problems; Appendix 2: Optimization Refreshers; Appendix 3: Some Results from Functional Analysis; Bibliography; Index*

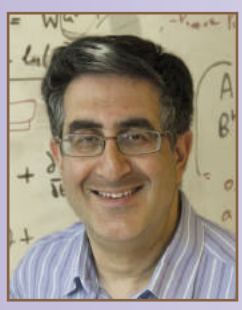
It has been a long time since I enjoyed so much reading a mathematical book. This book makes a delightful reading for researchers from the Computational Mechanics (CM) community with a reasonable amount of mathematical orientation and an interest in inverse problems (IPs). It has exactly the blend of rigorous analysis, practical examples and clear explanatory text that is very satisfactory, at least to my personal taste. In addition, it is written in a fluent, definitely non-dry style, despite the heavy technical content, which makes it an excellent reading material and not just a good reference text. The many examples and illustrations throughout the book contribute to its readability. Each chapter ends with a sequence of well-designed exercises.

The book does not intend to survey many known methods for solving IPs, but concentrates on a small number of general techniques, i.e., least squares, regularization, SVD and the adjoint method, which are useful for IPs in most application fields. The author "warns" the reader in the Preface that "this book is aimed at readers with rather substantial mathematical and scientific computing background, equivalent to masters in applied mathematics." Indeed, the book assumes more than basic knowledge in fields like linear algebra, PDEs, variational formulations, functional analysis and operator theory (e.g., compact operators play an important role here, and Appendix 3 gives a brief survey of results). Being aware of the high level of mathematics of engineering students in top schools in France, this warning may be intimidating for readers from other countries. Nevertheless, owing to the way the book is written, I believe that it will be accessible to many CM community members.

As defined on p.3, whereas "direct problems", which are the problems solved most of the time, seek the effects generated by given "causes", IPs seek the causes knowing the effects. *Figures 1 & 2* illustrate the setup of three IPs related to wave problems, i.e., determining the composition and geometry of the sea bottom, and determining the structure (voids, faults, etc.) and rock properties under the earth surface. Mathematically, IPs are notoriously difficult because they are typically ill-posed. Well-posedness includes three ingredients: existence (there exists a solution to the problem), uniqueness (there is only one solution) and stability (small changes in the data cause small changes in the solution). IPs almost always suffer from the lack of at least one of these ingredients.

The book comprises three parts. In the first part (chapters 1 and 2), the general properties of IPs are discussed and examples for various types of IPs are given. The examples include determining a past temperature field from measurements at present (which is a desperately unstable problem); finding the heat conductivity from partial temperature measurements; problems in hydrogeology (flow in porous media) such as determining the amount of pollution in the fluid, seismic exploration (as in *Fig. 2*); medical imaging; gravimetric prospecting; and ray tracing. The latter examples are described by an integral equation of the first kind, which is the prototype of linear IPs.





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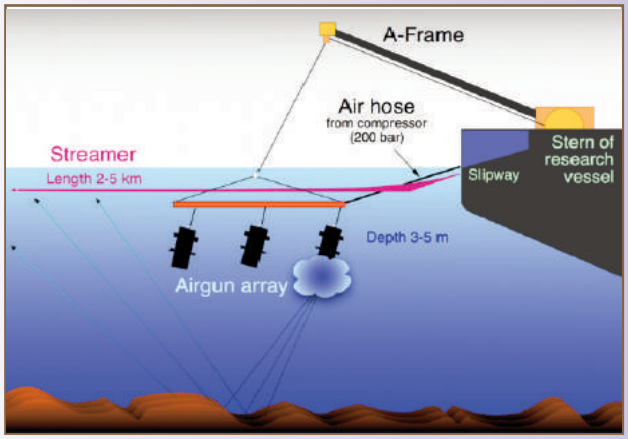


Figure 1:
Equipment used for marine seismic surveys. From Wikipedia, "Reflection seismology", by Hannes Grobe, Alfred Wegener Institute - Own work, sharing permitted.

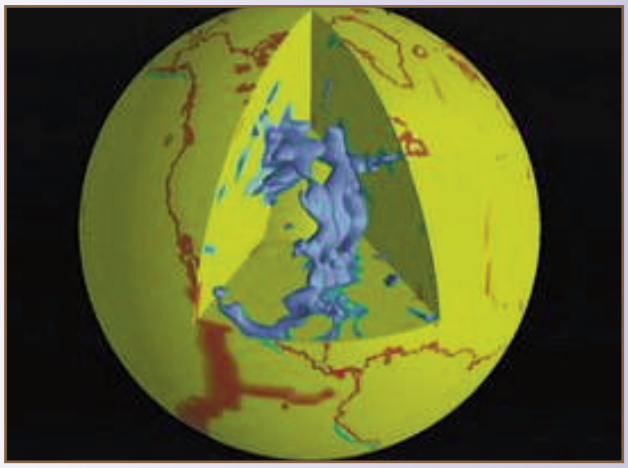


Figure 2:
NASA tomographic image of the subducted Farallon Plate in the mantle beneath eastern North America. From Wikipedia, "Seismic tomography", public domain.

The seismic exploration problem is described using the simplest model, namely the acoustic wave equation. Indeed, this is the first model used in solid-earth geophysics when testing a new solution approach. The models can become gradually more complicated and more realistic: linear elasticity in a homogeneous isotropic medium, heterogeneous medium, anisotropic medium, porous medium, etc. The author makes an interesting remark in this context: "it is not obvious that a refined model will be superior to the model we have just mentioned [i.e., the acoustic model]." Namely, if we do not have enough information (obtained by measurements) that would allow us to solve the IP, complicating the model (say, from acoustics to elasticity) may not be a good idea. While this is true, the author's conclusion that "our [acoustic] model may represent a reasonable compromise" may create the wrong impression that solid-earth geophysicists are content with acoustic models. In fact, geophysicists would rarely be satisfied from the results of this model alone; they would almost always solve later the more realistic IP problem of elasticity, while making sure that they have sufficient data for a successful solution.

Part 2 (chapters 3-5) concentrates on the integral-equation IP. The main motivating application is that of gravimetric prospecting, in which the densitiy of the rocks making up the earth structure is determined based on measurements of the earth's gravitational field. Two discretization methods for integral equations are described: quadrature collocation and Galerkin (the latter giving rise to a double integral). Then comes the realization that these methods, when applied directly to the IP, do not lead to convergence. In fact, the results become worse when refining the discretization. This is the outcome of the ill-posedness of the IP. The lesson is that one cannot attack head-on an ill-posed IP with standard solution methods.

Chapter 4 discusses the solution of least squares (LS) problems, which are at the heart of IPs, and the use of Singular Value Decomposition (SVD) to this end. Both the finite-dimensional case (matrices) and the infinite-dimensional case (operators) are discussed. The latter is much more complicated than the former, not just more technically involved. The SVD becomes SVE (E for Expansion) in the operator case.

One may raise the following question. In solving an IP, which is better: to first apply a solution method at the continuous level (operators) and only then to discretize and solve, or to discretize everything from the outset and then to apply a solution method at the discrete level (matrices)? This question, which, in fact, can be asked in various other contexts as well, is not discussed in the book. My tendency is to prefer the former, since I believe that it is best to postpone the discretization as much as possible. On the other hand, the latter approach may be easier to implement and requires less mathematical insight.

Chapter 5 discusses the important subject of regularization. Two common regularization methods are discussed: Tikhonov's method and spectral truncation. Regularizing an IP means converting the original ill-posed problem into a well-posed problem. The price of doing this is that one actually solves a different problem than the given IP, but hopefully a sufficiently similar one. As the author explains, we partly scarify accuracy in order to gain stability. This is nicely demonstrated by *Figure 3* (which is Fig. 5.1 in the book), where ε^2 is the Tikhonov regularization parameter and δ is the error in the data. If ε is too small, the problem is still very sensitive and the total error is large, whereas if ε is too large, the problem is overly regularized, which results in a large error. As the figure shows, there is a value of ε which is optimal. A nice discussion follows on how to pick the value of ε in practice, including a theoretical analysis and some examples. *Figure 4* (which is Fig. 5.2 in the book) shows that values between 10^{-3} and 1 lead to a good approximation. The chapter ends with a class of regularization methods based on iteration.

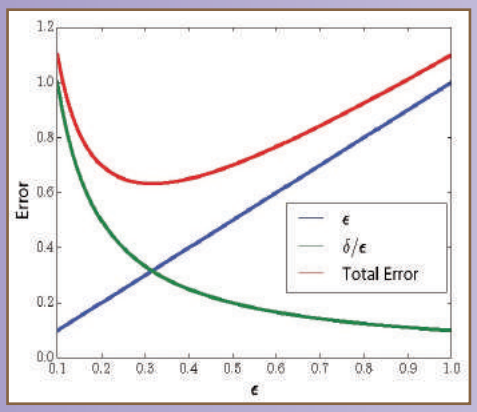


Figure 3:
The stability-accuracy tradeoff in regularization of IPs.
This is Fig. 5.1 in the book, p. 76

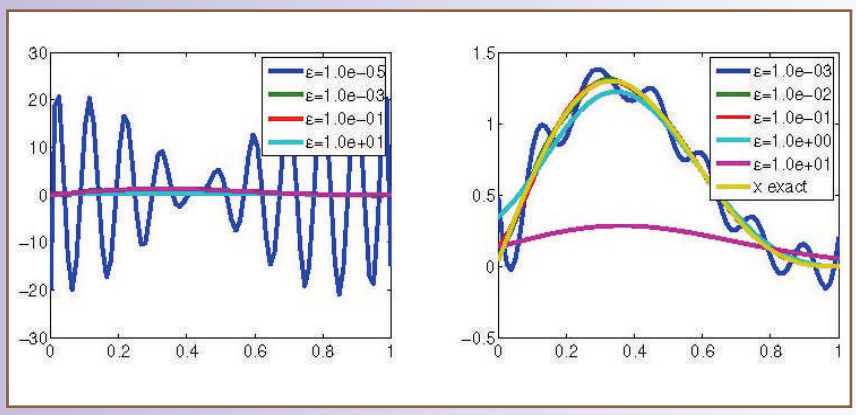


Figure 4:
Choosing the Tikhonov regularization parameter value.
This is Fig. 5.2 in the book, p. 81

Part 3 (chapters 6-8), which is beautifully written, deals with parameter identification problems. These IPs are typically governed by a PDE (or a system of PDEs), where the unknown 'parameter' is a coefficient in the PDE which may be a function of space and/or time. A reoccurring example is that of determining the (non-uniform) heat conduction based on temperature measurements. What makes the IP nonlinear is the nonlinear relation between the unknown parameter and the measurements. The theory about such problems is scarce, hence this part focuses on the numerical methods.

Chapter 6 focuses on the adjoint method, which is a variational method to calculate the gradient of the LS cost function in an efficient way. The author compares the adjoint method to the sensitivity method, which is a more straight-forward method but calculates the gradient less efficiently. Whereas the latter needs to solve the state (direct) problem N times per iteration, where N is the number of unknown parameters in the discrete problem, the adjoint method achieves the same goal by solving only two problems per iteration: a state problem and an adjoint problem. The latter is always linear, even if the state equation is nonlinear. The chapter includes, in addition to the natural derivation of the adjoint method by differentiating the state equation with respect to the parameter, a derivation based on the Lagrangian. I like this way of derivation less, since it has the disguise of a Lagrange multiplier method (LMM), whereas in fact it is not, since in the LMM the Lagrange multiplier is an unknown, and one cannot freely "choose" it to satisfy a certain relation, as is done here. The author is careful enough to call this "a trick".

Chapter 7 contains many examples for parameter estimation problems, employing the adjoint method. The optimization is done using the techniques described in Appendix 2, mainly BFGS and Gauss-Newton. Chapter 8 briefly discusses additional topics, most notably the statistic approach and Bayesian inversion.

Here and there, the text includes English oddities typical to French speaking scientists, like derivation instead of differentiation (p. 7), note instead of denote (p. 11, p. 49), 'as soon as' instead of 'as long as' (p. 33), still instead of again (p. 40), definite positive instead of positive definite (p. 51, p. 187), application instead of mapping (p, 111), 'the condition is verified' instead of 'the condition is satisfied' (p. 189), and even 'et' instead of 'and' (p. 188). These slight mistakes are completely harmless, and some would say that they are even charming (like speaking English in a French accent).

More serious than this, unfortunately, are the many typos scattered in the text and the equations. I will mention only one example out of many: in eq. [2.14], the third equation includes a vector term which should be scalar (the divergence). Incidentally, the IP described in relation to eq. [2.14] does not make much sense, since it is obtained by omitting some information from the well-posed direct problem without compensating this omission by any extra information. Despite the slight inconvenience caused by the many typos, this should not deter one from reading this excellent book. Hopefully the author will publish an errata list, and a better proofing job will be done for the second edition.

In summary, this is a highly recommended book for CM researchers who are interested in inverse problems or wish to be introduced to the subject. ●

Symposium to Honor Professor Thomas JR Hughes on his 75th Birthday at WCCM 2018

by
Arif Masud
Yuri Bazilevs
Alessandro Reali
Wing-Kam Liu

The 13th World Congress on Computational Mechanics was held in New York City on July 22-27, 2018. A highlight of the conference was a symposium dedicated to honoring Professor Thomas JR Hughes at the occasion of his 75th birthday. This special symposium was a tribute from friends, colleagues, former students and associates of Tom Hughes to his numerous pioneering contributions to the field of Computational Mechanics, and for his leadership in establishing Computational Mechanics as a fundamental Discipline in Engineering and Sciences. This event was organized by a committee comprised of former students of Professor Hughes that included Arif Masud, Wing Kam Liu, Isaac Harari, Yuri Bazilevs, Alessandro Reali, and Greg Hulbert.

The symposium had nine sessions that were loosely grouped into themes that represented the wide spectrum of Tom's contributions to the field. It had a strong line-up of speakers, ran from Monday to Wednesday, and attracted a large audience. Sessions included talks from friends, colleagues, former students and associates of Tom and reflected the contributions he made directly, the contributions he made through the students he trained and associates he guided, and the contributions made by friends and colleagues he inspired. Talks also contained memorable photos and anecdotes from Tom's personal and professional life. Yuri Bazilevs composed and, as part of his presentation, recited a poem in honor of Tom titled "Ode to TJR Hughes":

Figures Top and Right:
Symposium presentations

Among the three "T" 's
Of Computational Mechanics,
Two are in Texas,
And one is in the Heavens.

TJR Hughes, in "The City" born and raised,
Left for the Golden State, quite un-phased.
He found himself in a progressive's nest,
And challenged some FEM problems left unaddressed.

Then, shells stopped locking,
Contact started working,
Time marching was enabled,
And fluids got stable!

Bay Area tech bubble
Brought in minor trouble.
Yet Texas came kneeling,
And… CAD needed healing.

Thus, IGA was born,
And, to much scorn,
After many persuasions,
It accrued some citations.

So, is it Math or Engineering?
It's in BOTH that we are hearing
Impact great and so far reaching,
The naysayers can't stop bitching.

But, no resting on the laurels,
No time to count the cash,
Keep living for tomorrow,
And make another splash!

The three-day birthday symposium culminated in a reception and banquet that were generously sponsored by the Livermore Software Technology Corporation (LSTC).

At the banquet Tom was presented with a "Book of Comments" from his friends, students, and collaborators, about his research and what it meant to them personally and for the field of mechanics in general. Elizabeth Hughes, Tom's youngest daughter, did a fantastic job in putting the book together and adding pictures of the Hughes family that gave it a personal touch. At the closing of the event, Wing Kam Liu, Arif Masud, Yuri Bazilevs, JS Chen, and Alessandro Reali spoke on behalf of Tom's groups at Caltech, Stanford, Austin, students of Tom's close friend and collaborator Ted Belytschko, and students and colleagues from Tom's group who are now in Europe. Tom also gave a touching speech, and expressed his gratitude to everyone who made his 75th birthday celebration so memorable. ●

Figures Top and Left:
Symposium banquet

Two Priority Programmes Related to GACM by the German Research Foundation (DFG)

"A particular feature of the Priority Programme is the nationwide collaboration between its participating researchers. The DFG Senate may establish Priority Programmes when the coordinated support given to the area in question promises to produce particular scientific gain. As a rule, Priority Programmes receive funding for a period of six years." [http://www.dfg.de/en]

SPP 1897: Calm, Smooth and Smart – Novel Approaches for Influencing Vibrations by Means of Deliberately Introduced Dissipation

In 2015, the German Research Foundation (DFG) has approved a Priority Programme (SPP), entitled "Calm, Smooth and Smart – Novel Approaches for Influencing Vibrations by Means of Deliberately Introduced Dissipation". The programme is scheduled to run for six years. The joint work in the Priority Programme started with a kick-off meeting in September 2016 and end of 2019 the second funding phase will start.

The aim of achieving a "calm, smooth and smart" behaviour of technical systems is driven forward by an interdisciplinary group of about 15 closely cooperating projects from the fields of mechanics, mathematics, control theory, tribology, fluid mechanics, and material sciences. In this context, "calm" represents the demand to avoid or at least to severely reduce unwanted noise, "smooth" ensures a still comfortable and jerk free operation, and "smart" means that the introduced damping devices not only help to achieve the desired vibrations behaviour, but also that they take over additional functional tasks. This contributes to the urgent needs of innovative approaches to minimize the vibrations of the increasing number of lightweight constructions. Since there is only a limited knowledge on most physical dissipation phenomena available, one focus is on the understanding and modelling of damping phenomena and damping devices, making it possible to take dissipative effects into account in early design states. Another focus is led on numerous practical applications. For example, the reduction of brake squeal reduces the noise pollution for humans and the environment or particle dampers can reduce vibrations over large frequency ranges.

Coordinator: **Prof. Peter Eberhard, Stuttgart**
Homepage: **www.itm.uni-stuttgart.de/spp_css**

SPP 2020: Cyclic deterioration of High-Performance Concrete in an Experimental-Virtual Lab

The Priority Program SPP 2020 started in June 2017 with scientists from thirteen Universities with overall twelve research projects.

Nowadays, modern high-performance concrete allows even lighter, more filigree and resource-efficient structures which, however, are more susceptible to vibrations due to their reduced dead weight.

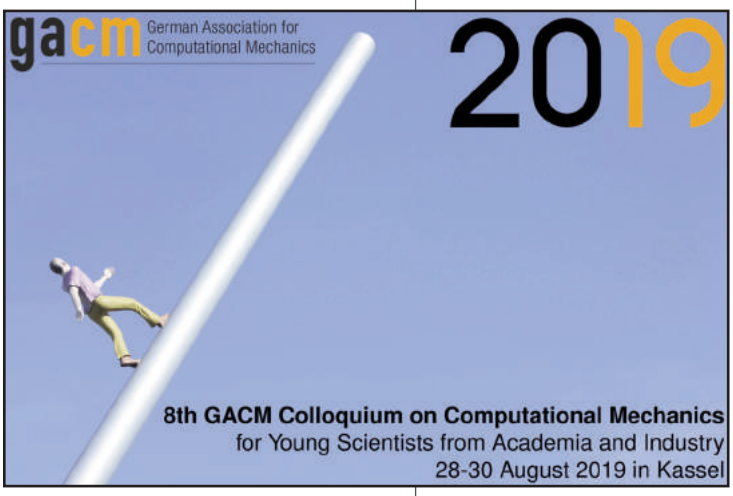
Structures and components – such as long-span bridges for high-speed trains, wind-power plants and machine foundations – are also typically subjected to very large variable loads and very high numbers of load cycles. The fatigue behavior of high-performance concrete is decisive for the successful design and the realization of such applications. The designed aim of this program is to capture, understand, describe, model and predict the material degradation of high-performance concrete using the newest experimental and virtual numerical methods. Since the damage processes occur on a very small scale, they cannot be entirely observed during the load tests. Therefore, the desired results are developed from a close cooperation between the material science and the numerical mechanics knowledge, which is the interconnection of experiment and computation in an Experimental-Virtual-Lab. The material degradation can be observed through the multiscale numerical-models calibrated on the basis of suitable damage indicators recorded during the experiments. Besides the classical macroscopic fatigue tests, these indicators are selected among modern measuring technology and microstructural investigations like Ultrasonic Analysis, Computer Tomography, REM und TEM-Microscopy, whose recording makes the already time-consuming fatigue test a demanding issue.

The numerical-modelling description of the heterogeneous concrete microstructure as well as the damage and crack developing at different scale levels over several hundreds of load cycles present particular research challenges in this priority program. To this extent, some numerical methods used are Finite Element, Voxel FE, Interface FE, Bonded-Particle Model, XFEM, whereas the crack developing is described, for example, through Phase Field Theory, Cohesive Interface Models, Continuum Damage Mechanics and Fracture-Based Plasticity Approach. Finally, in some cases, multifield models are developed in order to consider the interaction with the temperature or water flow field with the mechanic field.

Coordinator: **Prof. Ludger Lohaus, Hannover**
Homepage: **www.spp2020.uni-hannover.de**

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. It intends to bring together young scientists who are engaged in academic and industrial research on Computational Mechanics and Computer Methods in Applied Sciences.

For further information, please see the conference webpage:
www.uni-kassel.de/go/gacm2019

Chinese Conference on Computational Mechanics 2018
in conjunction with
International Symposium on Computational Mechanics 2018
successfully held in Nanjing, China
August 19-23, 2018

Chinese Conference on Computational Mechanics 2018 (CCCM2018) and International Symposium on Computational Mechanics 2018 (ISCM2018) were successfully held at Nanjing, China on August 19-23, 2018. The CCCM-ISCM 2018 was organized by Chinese Association of Computational Mechanics (CACM) and was locally organized by Hohai University and Jiangsu Society of Theoretical and Applied Mechanics. Prof. Zhuo Zhuang from Tsinghua University, Prof. Yao Zheng from Zhejiang University, and Prof. Qing Zhang from Hohai University, were co-chairs of the conference.

This conference was mainly aimed to promote the comprehensive and deep academic exchanges and discussions on the research and applications of computational mechanics both in China and around the world. More than 700 delegates from China, US, UK, Australia, Germany, France, Singapore, etc. attended the conference. This conference received 549 abstracts, set up 68 parallel sessions covering 29 topics, and set 550 oral reports including 17 plenary lectures.

The opening ceremony of the conference was presided by Prof. Qing Zhang and Prof. Hui Xu, the President of Hohai University, delivered a welcome speech on behalf of the local organizer. Prof. Zhuo Zhuang, the President of CACM, delivered a welcome speech on behalf of the organizer.

Figure 1:
Prof. Qing Zhang, the Co-Chair of the conference presided the opening ceremony

Figure 2:
Prof. Hui Xu, the President of Hohai University delivered a welcome speech on behalf of the local organizer on the opening ceremony

Prof. Wanxie Zhong, the academician of Chinese Academy of Sciences, from Dalian University of Technology, China, Prof. Wing Kam Liu, the Chairman of International Association of Computational Mechanics (IACM), from Northwestern University, USA, Prof. Chuanzeng Zhang, Member of the European Academy of Sciences and Arts, from Siegen University, Germany, Prof. Chongmin Song, from University of New South Wales, Australia, Prof. Fangsen Cui, from Institute of High Performance Computing, Singapore, Prof. Zhiqiang Feng, from University of Evry, France, Prof. Qingping Sun, from The Hong Kong University of Science & Technology, Hong Kong, China, Prof. Chenfeng Li, from Swansea University, UK, Prof. Hongwu Tang from Hohai University, China, Prof. Jiun-Shyan Chen from University of California, San Diego, USA, Prof. Guirong Liu from University of Cincinnati, USA, Prof. Shaofan Li from University of California, Berkeley, USA, Prof. Song Fu from Tsinghua University, China, Prof. Xikui Li from Dalian University of Technology, China, Prof. Bo Wang from Dalian University of Technology, China, Prof. Dongdong Wang from Xiamen University, China, Prof. Yao Zheng from Zhejiang University, delivered the plenary lectures, respectively.

During the CCCM-ISCM2018 conference, the awarding ceremony for three awards was held. The CACM Life Achievement Awards were granted to

Prof. Wanxie Zhong, Dalian University of Technology, Porf. Junzhi Cui, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Prof. Mingwu Yuan, Peking University, and Prof. Zhenhan Yao, Tsinghua University. Winners of the Achievement Award and the Young Investigator Award of the 5th Qian Ling-Xi Awards for Computational Mechanics were Prof. Yao Zheng, Zhejiang University and Prof. Bo Wang, Dalian University of Technology, respectively. ●

by
Qing Zhang, Lie Wang, Zhuo Zhuang

Figure 3:
Prof. Zhuo Zhuang, the Chairman of CACM, delivered a welcome speech on behalf of the organizer on the opening ceremony

Figure 4:
Prof. Yao Zheng delivered the plenary lecture

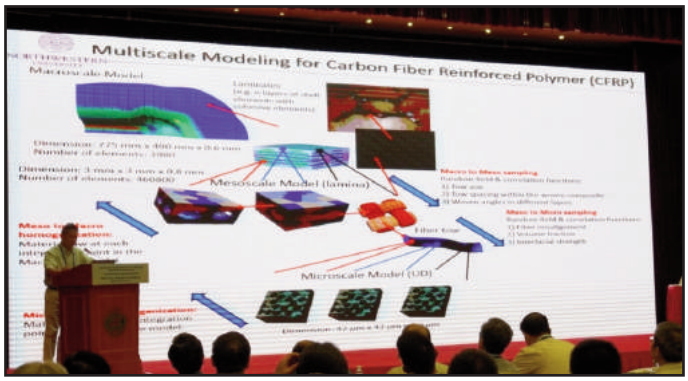


Figure 5:
Prof. Wing Kam Liu delivered the plenary lecture, who is the Chairman of International Association of Computational Mechanics (IACM), from Northwestern University, USA

Figure 6:
Prof. Wanxie Zhong delivered the plenary lecture, who is the academician of Chinese Academy of Sciences, from Dalian University of Technology, China

Figure 7:
Picture of the conference room

Figure 8:
Picture of the conference room

- Trends and activities of JSCES -

On behalf of the Japan Society for Computational Engineering and Science (JSCES), I would like to introduce the recent trends and activities as the Japan's biggest organization in the field of computational mechanics.

First of all, the JSCES renewed the Executive Council in May 2018 after the elections, which is formed by the following members (two-year term in the JSCES's bylaws): T. Yamada (Yokohama NU, President), M. Fujisaki (Fujitsu, Vice-President), K. Yuge (Seikei U, Vice-President), J. Matsumoto (AIST, Secretary General), S. Fujikawa (Mazda), S. Hagihara (Saga U), H. Hasegawa (Shibaura IT), D. Isobe (U Tsukuba), J. Kato (Nagoya U), H. Miyachi (Tokyo City U), K. Nagano (Mizuho IR), T. Nagashima (Sophia U), S. Nishiwaki (Kyoto U), S. Okazawa (U Yamanashi), M. Sakuraba (Nippon Koei), H. Sakurai (Shimizu), R. Shioya (Toyo U), M. Takagaki (RTRI), N. Yamasaki (NSSMC), H. Watanabe (MSC), K. Terada (Tohoku U, inspector), Y. Umezu (JSOL, inspector).

Figure 1: Prof. Takahiro Yamada, the President of JSCES

At present, the JSCES has 1085 individual members and 82 corporate members. The individual members come from 60% of universities and research institutes and 40% of industries. In recent years, the Executive Council has been devoting much effort to increase corporate members and individual members belonging to industries. For one of such activities, benefits of corporate membership are clarified and widely disseminated. Moreover, the Research Committee of JSCES operates Study Groups for HQC (High Quality Computing), PSE (Problem Solving Environment), Hypercomplex Disaster Simulation, Modeling and Simulation Methods of Uncertainties, Benchmarks, Education of Computational Mechanics, Development of Model Base of Automobile Structures to exchange information among the members and cooperation between academia and industries.

by: ***Takahiro Yamada*** *- Figure 1*

Summer Camp for Students

"The summer camp for students 2018", a successful series hosted by JSCES from 2013, was held during September 8-9, 2018. This year, 24 students from various universities throughout Japan gathered in Nagatoro, which is a scenic town in the mountains of Saitama Prefecture (*Figure 2*). During this camp, 17 students presented their ongoing researches, and five keynote speakers gave talks on their

Figure 2: Participants of the JSCES summer camp for students 2018

research experiences in universities, national laboratories and industry (*Figure 3*). The best presentation awards were given to three students (Mr. Nakayama, Mr. Aida and Mr. Tezuka) from Prof. Yamada, the President of JSCES (*Figure 4*). Attendees enjoyed a barbeque dinner after the lecture meeting and built good relationships through communication in a relaxed atmosphere.

by: ***Naoto Mitsume***

Figure 3:
Lecture meeting in a mountain cottage in Nagatoro

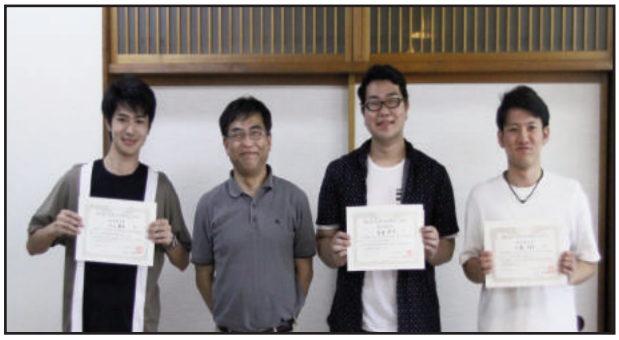


Figure 4:
Winners of the best presentation awards (from left to right, Mr. Nakayama, Prof. Yamada, Mr. Aida and Mr. Tezuka)

Study Group on Automobile Structural Model-Based Development

There are segmentation design items for automobile development. Performance evaluations have achieved large progress in experimental and computational simulation. Deriving a multipurpose optimum solution with plural objective functions of the performance evaluation will be indispensable in future. In addition, by introducing initial design, costs and the other various constraint conditions, these optimizations should be extended to effective automobile model-based development. In the above background, this study group establishes a cross-field academic research organization. The current number of members is approximately 30, including industrial, academic and government researchers.

The main event is exchange of ideas, opinions, problems and technologies of automobile structural model-based development for researcher, engineers and students in automobile development, computational science and engineering, mathematics, and so on. In annual conference of JSCES, this study group provides an organized session for discussing ideas on recent advances in areas related to computational methods, numerical modelling for automobile model-based development (Figure 5).

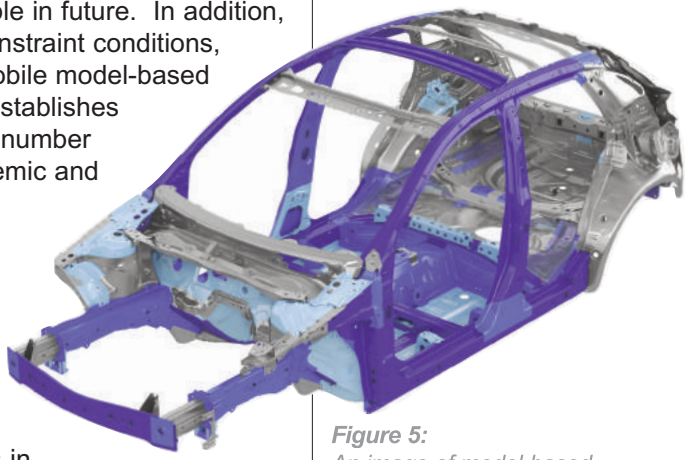


Figure 5:
An image of model-based development of automobile frame

by: ***Shigenobu Okazawa***

Prof. Yoshiaki Yamada

Prof. Yoshiaki Yamada passed away in Tokyo, Japan on June 26, 2018, in his age of 96. He was one of the leaders and pioneers of nonlinear finite element method society. One of the largest achievements in his career was development and implementations of elasto-plastic constitutive equations in finite element methods. The outcomes have been widely used in various commercial codes and have helped to investigate physical phenomena and to create numerous product designs. We express our deep and sincere condolences to his family (*Figure 6*). ●

Figure 6:
Prof. Yoshiaki Yamada (the fourth from left in the front row) with his colleagues

For all inclusions under ***JACM*** *news please contact:*
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The Japan Association for Computational Mechanics (JACM) is a union of researchers and engineers working in the field of computational mechanics mainly in Japan. JACM is a loosely coupled umbrella organization covering 29 computational mechanics related societies in Japan through communication with e-mail and web page (https://ja-cm.org/index-e.html). The number of individual members is about 310. JACM members actively participate the IACM activities.

On July 25th, 2018, the 2018 JACM annual meeting and award ceremony were held on the occasion of the WCCM XIII and PANACM II, New York, USA (*Figure 1*). In the award ceremony, the award winners received their certificates from Prof. H. Okada (President of JACM, *Figure 2*). The other award winners are presented with their photographs (*Figures 3 and 4*).

Figure 1: *2018 JACM annual meeting group photo*

In 2018, The JACM Computational Mechanics Awards which are the highest awards were presented to Profs. Chisachi Kato (UTokyo), Kikuo Kishimoto (Tokyo Inst. Tech.) and Yoji Shibutani (Osaka Univ.). The JACM Fellows Awards were presented to Profs. Yohsuke Imai (Osaka Univ.), Takayuki Yamada (Kyoto Univ.) and Tomonori Yamada (UTokyo). The JACM Young Investigator Award were presented to Profs. Kazuya Shibata (UTokyo), Takahiro Tsukahara (Tokyo Univ. Science) and Tinh Quoc Bui (Tokyo Inst. Tech.).

Figure 2: *JACM Award for Young Investigators in Computational Mechanics winners with Prof. H. Okada in the award ceremony (a) Prof. Kazuya Shibata (UTokyo), (b) Prof. Takahiro Tsukahara (Tokyo Univ. Science) and (c) Prof. Tinh Quoc Bui (Tokyo Inst. Tech.)*

(a) *(b)* *(c)*

Figure 3: *Computational Mechanics Award: (a) Prof. Chisachi Kato (UTokyo), (b) Prof. Kikuo Kishimoto (Tokyo Inst. Tech.) and (c) Prof. Yoji Shibutani (Osaka Univ.)*

(a) *(b)* *(c)*

At the annual meeting, the JACM members discussed the current state of the JACM and future plans and events such as APCOM VII in Taipei, held in December 2019 and COMPSAFE2020 (3rd International Conference on Computational Engineering and Science for Safety and Environmental Problems, an APACM Thematic Conference & IACM Special Interest Conference) in Kobe, Japan, held in March 2020.

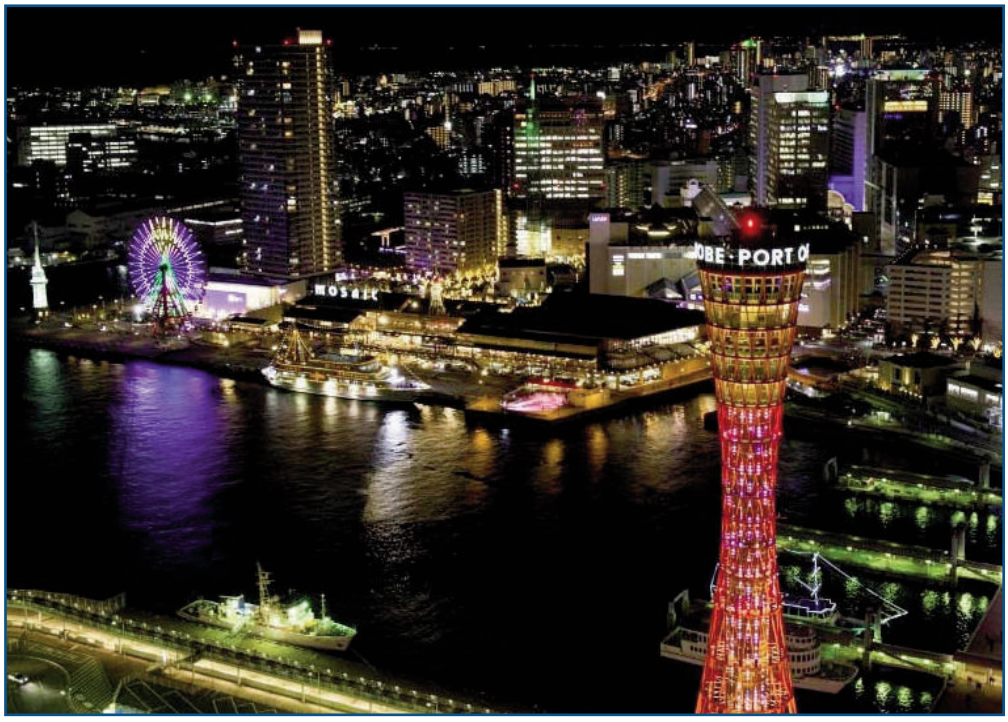
(a) (b) (c)

Figure 4:
Fellows Award:
(a) Prof. Yohsuke Imai (Osaka Univ.),
(b) Takayuki Yamada (Kyoto Univ.)
and (c) Tomonori Yamada (UTokyo)

Upcoming Events

The JACM and JSCES (The Japan Society for Computational Engineering and Science) will jointly host the **3rd International Conference on Computational Engineering and Science for Safety and Environmental Problems (COMPSAFE2020)** which will be held during **March 8-11, 2020**, in Kobe, Japan (Figure 5). This conference series is an APACM Thematic Conference and an IACM Special Interest Conference, aimed to bring together researchers and scientists from all over the world, who fight daily in the field of disaster prevention and mitigation, structural and material failure, safety and security maintenance, and so on.

Please note that the minisymposium proposal and the abstract submission are due on June 30, 2019 and October 31, 2019, respectively. For further information, please check www.compsafe2020.org. ●



Figures 5:
A night view of Kobe. (© KOBE TOURISM BUREAU)

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A Tale of Two Conferences

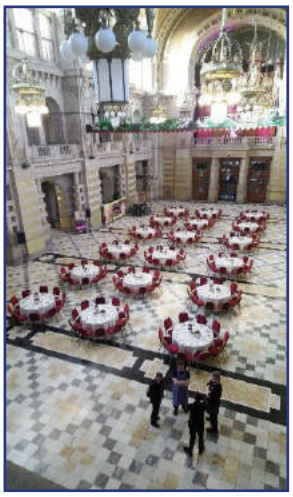

Figure 1: *Glasgow Appreciation Dinner Venue*

Figure 2: *Mané Harutyunyan presenting at the Science Slam, Glasgow*

Only a few weeks apart this summer, I attended two major conferences: **WCCM** in New York and the **ECCOMAS ECCM-ECFD** Conference in Glasgow. I don't think we have too much to worry about in terms of interest in our area, given the large numbers of participants. At Glasgow over 1900 attended from 52 different countries, including 656 students. In New York the attendance was much higher. Both events were well-organised and I'd like to highlight an innovative feature of each.

In Glasgow, as well as an outstanding Appreciation Dinner at Kelvingrove Art Gallery (left), one of the evenings was enlivened by a "Science Slam" which took place in a converted church close to the University. This was not an event to arrive at without a sense of humour as it was an opportunity for established academics and students to show their informal side, by trying to explain an aspect of their research, or to pose a provocative question, to an audience in an atmosphere akin to a comedy club. I still have no full answer to the question posed by one of Computational Mechanics's leading stars … "What is a Tree?"

In New York I was gripped by the "Visionary Talks" which were held at lunchtimes during the conference. I managed to see two, from leading women in science and engineering, who talked eloquently about their journey to their current position, the challenges they had met on the way and their visions for education in engineering.

It is to be hoped that innovations like these are repeated at future conferences of IACM and ECCOMAS.

All change at UKACM

My three-year term as President of UKACM comes to an end this December and I am delighted to inform readers that **Dr Rubén Sevilla** of Swansea University is to be the next President. I am confident he will continue to raise the profile of the UK in IACM and other organisations and wish him well.

Join us for our annual conference in London this April!

*From the Conference Chair: **Professor Roger Crouch,** Dean of the School of Mathematics, Computer Science and Engineering*

The **27th Annual UKACM conference** will take place on **10-12 April 2019** at City, University of London. The venue will be in the heart of London, at the University's Northampton Square Campus, to the north of the Clerkenwell's highly-creative design district. We very much look forward to being your hosts in the capital city and strongly encourage you all to join us for the conference dinner on the 11th April.

The 2019 UK conference will provide the opportunity for researchers in the rich and extraordinarily successful field of computational mechanics to: (i) present and their most recent innovations, (ii) exchange ideas with colleagues and (iii) explore collaborative research opportunities. The gathering follows the fine tradition of annual meetings started in Swansea in 1993. We warmly welcome all; most particularly early-career researchers who are perhaps studying for their MRes/MPhil/PhD, but have yet to showcase their findings to a wider audience. The scope will encompass not just solid and fluid mechanics, but also the underpinning numerical methods for efficient large scale computation, error analysis and optimisation. In 2019 we might expect to see contributions that link new developments in AI/machine learning to computational mechanics. The programme for the 3-day conference will be announced in the autumn of 2018 so please look out for the call for papers. ●

GIMC & GMA Meeting in Ferrara

The AIMETA Computational Mechanics and Material Groups (GIMC & GMA) are pleased to announce that the conference GIMC-GMA 2018, held in Ferrara on September 13-14 2018, was very successful and had a large turnout:

- Over 120 participants, from Italian and foreign Universities;
- Over 95 presentations organized in parallel GIMC and GMA sessions;
- Two invited lectures given by Professor Franco Brezzi and by Professor Marino Arroyo;
- A special session devoted to the presentation of the PhD theses in Computational Mechanics and in Mechanics of Materials winner of the GIMC and GMA awards.
- A special session in honor of Professor Antonio Tralli.

Details on the meeting can be found at the web site
https://gimc2018.sciencesconf.org/

GIMC Best PhD Thesis Award

The GIMC Best PhD Thesis Awards committee, composed by Paolo Bisegna (Roma Tor Vergata University), Stefano De Miranda (Bologna University), and Alessandro Veneziani (Emory University, Atlanta, USA), selected the following thesis defended during the 2017 year:

- **Dr. Paolo Di Re**, La Sapienza University of Roma, *"3D beam-column finite elements under tri-axial stress-strain states: non-uniform shear stress distribution and warping"* for the Computational Solid Mechanics Award
- **Dr. Francesco Fambri**, Trento University, *"Discontinuous Galerkin methods for compressible and incompressible flows on space-time adaptive meshes"* for the Computational Fluid Mechanics Award.

Previous recipients of the GIMC Best PhD Thesis Award are:

2017 **Nicola Nodargi** Incremental energy minimization and mixed finite element formulations for the analysis of inelastic structures (Solids)
2017 **Andrea Montanino**, The modified finite particle method in the context of meshless methods (Fluids)
2016 **Davide Grazioli**, Multiscale and multiphysics modeling of Li-Ion battery cells (Solids)
2016 **Walter Boschieri**, High order direct arbitrary-lagrangian-eulerian (ALE) finite volume schemes for hyperbolic systems on unstructured meshes (Fluids)
2015 **Giulia Scalet**, Shape memory and elastoplastic materials: from constitutive and numerical to fatigue modeling
2014 **Rossana Dimitri**, Isogeometric treatment of large deformation contact and debonding problems with NURBS and T-splines

Thematic Conference on Meshfree and Particle Methods: Applications and Theory

Conference Website: http://mfpm2018.usacm.org

The USACM Thematic Conference on Meshfree and Particle Methods: Applications and Theory was held at the historic La Fonda on the Plaza in Santa Fe, New Mexico, **September 10-12, 2018**. The conference was supported by the Technical Thrust Area (TT) of USACM on Novel Methods in Computational Engineering and Science and organized by Jacob Koester and Joe Bishop (Sandia National Laboratories), Duan Zhang (Los Alamos National Laboratory, Deborah Sulsky (University of New Mexico), and Bo Li (Case Western Reserve).

Figure 1: *Beginning of a technical session in La Fonda on the Plaza*

The conference sought to build a stronger connection between the computational mechanics communities working on novel methods and the communities working on applications and experimentation. The exchange of ideas enriched method development by cross-pollinating ideas between various computational methods by keeping researchers informed on the current application needs. The following focus areas were a part of the program: Penetration and Perforation, Shock and Hydrodynamics, Advanced Manufacturing, Rapid Design-to-Analysis, Geoscience and Natural Disasters, Fluid-Structure Interaction and Other Coupled Problems, Multi-Scale, Implementation and High-Performance Computing, Mathematical Theory and Method Development, Comparison of Related Methods, and Damage and Fracture.

With nearly 90 attendees, the Thematic Conference featured five Plenary Lectures (delivered by Steve Attaway, Jerry Brackbill, Sergio Idelsohn, N. Sukumar, and Dondong Wang), 70 talks and 22 posters by students and post-doctoral fellows during an informal poster session. Participants were also able to network during an opening reception, lunch, breaks and the conference banquet which featured Joseph Teran, who presented an entertaining use of particle methods in movie animation.

The Organizers would like to thank all the Thematic Session organizers and the conference participants for their efforts in delivering a high-quality technical program. ●

Figure 2: *Plenary speaker Jerry Brackbill presenting*

Figure 3: *Conference dinner*

Figure 4: *Poster session presenters*

USACM Upcoming Events

further details at usacm.org

- ***15th U.S. National Congress on Computational Mechanics***
  Austin, TX, July 28-August 1, 2019; **http://15.usnccm.org**
- ***Uncertainty Quantification in Computational Solid and Structural Materials Modeling***
  Baltimore, MD, January 17-18, 2019; **http://uq-materials2019.usacm.org** (TTA on Uncertainty Quantification)
- ***Topology Optimization Roundtable***
  Albuquerque, NM, March 10-13, 2019; **http://paulino.ce.gatech.edu/TopOpt%20Workshop%20Website/** (TTA on Large Scale Structural Systems and Optimal Design) ●

IGA 2018:
Isogeometric Methods – Integrating Design and Analysis

Conference Website: http://iga2018.usacm.org/

October 10th to 12th, 2018, the third ICES (Institute for Computational Engineering and Sciences) and USACM (United States Association for Computational Mechanics) Thematic Conference, IGA 2018: Isogeometric Analysis: Integrating Analysis and Design, was held at the outstanding AT&T Conference Center (http://www.meetattexas.com) on the campus of the University of Texas at Austin. The local organizer and conference chair was Tom Hughes. The Steering Committee consisted of Ferdinando Auricchio, Yuri Bazilevs, David Benson, Tor Dokken, Trond Kvamsdal, Alessandro Reali, and Jessica Zhang.

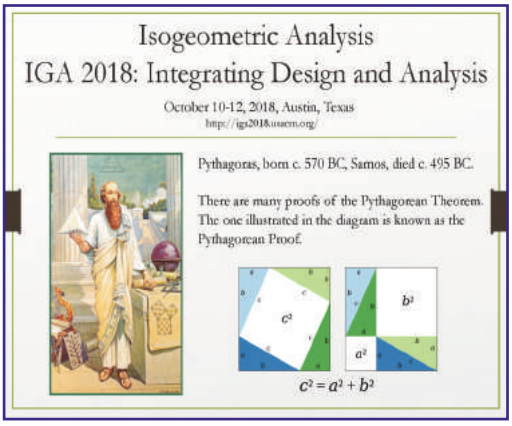

Figure 5:
Conference Poster

Despite hurricane Michael at the time in the United States, which severely impacted air travel, the conference was very well attended. There were 150 registrants including 46 doctoral and 8 post-doctoral students. Expanding the format of the first two conferences in Austin in 2011 and 2014, there were 122 presentations of one-half hour each, and three simultaneous parallel sessions on October 10th and four simultaneous parallel session on both October 11th and 12th. In addition, for the first time, an Industrial Panel discussion was held, with 28 representatives from 15 companies that attended from the finite element analysis industry, as well as end user, preprocessor, mesh generation, and computational model development companies. A student/postdoc poster competition, sponsored by Corefrom, LLC, was held and there were 12 entries. Professors Bjorn Engquist and Omar Ghattas served as judges. The three winners, who received award certificates and cash prizes, were:

First place, $1,000, **Mattia Tani, University of Pavia**:
"The wonders of continuity: When C^{p-1} IGA is faster than C^0 FEA"
Second place, $500, **Aishwarya Pawar, Carnegie Mellon University**:
"DTHB3D_Reg: Dynamic Truncated Hierarchical B-splines Based 3D Nonrigid Image Registration"
Third place, $250, **Roel Tielen, Delft University of Technology**:
"Efficient p-Multigrid Methods for Isogeometric Analysis."

The conference was highlighted by considerable time for the attendees to interact and exchange ideas during extended breaks, organized breakfasts and lunches each day, and enjoyable social events, including a welcome reception the night before the conference, a reception during the poster competition the first evening of the conference, a gala banquet the second evening, and a closing dinner the third night.

Isogeometric Analysis has become a focal point of research in the CAGD (Computer Aided Geometric Design) and FEA (Finite Element Analysis) communities, and now has gained considerable traction in industry. It was clear from the many excellent presentations that incredible progress has been made and that the goal of Isogeometric Analysis, to fully integrate geometric design and engineering analysis, and thereby eliminate an enormous bottleneck in product development presently accounting for more than 80% of overall analysis time, is well on its way to being achieved. ●

Thomas J.R. Hughes
Austin, October 15, 2018

Figure 6:
Tom Hughes and the poster contest prize winners. From left to right, Roel Tielen, Tom Hughes, Mattia Tani, and Aishwarya Pawar.

Figure 7:
The Austin, Texas skyline, site of IGA 2018

Israel Association for Computational Methods in Mechanics

During the past year the Israel Association for Computational Methods in Mechanics (IACMM) held two symposia. The 43rd Israel Symposium on Computational Mechanics (ISCM-43) was held in Oct 2017 at Tel-Aviv University, organized by Profs. Isaac Harari and Slava Krylov. The interesting opening lecture was given by the international invited speaker Prof. Manfred Bischoff from the University of Stuttgart, Germany, titled “Rotation-free parameterization and isogeometric discretization of shear deformable shells”. *Figure 1* shows Prof. Bischoff lecturing. The symposium included 11 other lectures, presented by practitioners and researchers from industry and academia. These included among others talks by Prof. Slava Krylov (Actuation of higher harmonics in large arrays of micromechanical cantilevers for expanded resonant peak separation), Prof. Yair Shokef (Geometrically frustrated mechanical metamaterials) both from Tel Aviv University, Dr. Pavel Trapper (Unified numerical analysis of pipe-lay on a seabed with nonlinear stiffness), from Ben-Gurion University and Dr. Regina Katsman (Fracture-driven methane bubble ascent within shallow fine-grained clay-bearing aquatic sediments: dynamics and controlling factors) from the University of Haifa. *Figure 2* shows Prof. Krylov during his talk. Ms. Dana Bishara, a PhD student of Prof. Mahmood Jabareen from the Technion was the winner of the ISCM-43 competition for the best presentation – the title of her talk was "An advanced finite element formulation for modeling electro-active polymers". *Figure 3* is a group photo of the Invited speaker with the IACMM executive council.

The 44th IACMM Symposium was held in March 2018 at the Ben-Gurion University, organized by Prof. Erez Gal and Dr. Yuri Feldman. The delightful opening lecture was given by the international invited speaker Prof. Stefan Hartmann from the Clausthal University of Technology, Germany, titled “Two decades of the method of

Figure 1: *Prof. Bischoff delivering the invited lecture at the ISCM-43, Oct 2017, TAU, Tel-Aviv*

Figure 2: *Prof. Slava Krylov during his talk at ISCM-43*

Figure 3: *Group photo of IACMM executive council and international speaker at ISCM-43, at the Tel-Aviv University. Left to Right (Up): Z. Yosibash, J. Tal (Down): D. Givoli, A. Herszage, I. Harari, M. Bischoff, M. Jabareen, P. Bar-Yoseph, S. Krylov*

Figure 4:
Hartmann delivering the invited lecture of the ISCM-44, March 2018, Ben-Gurion University

Figure 5:
Dr. Yaniv Brick the winner of the ISCM-44 best presentation, during his talk

vertical lines in non-linear finite elements". Prof. Hartmann also gave a tutorial on "Aspects of material parameter identification in solid mechanics". *Figure 4* shows Prof. Hartmann lecturing and answering questions. Nine additional presentations were given at ISCM-44, including a talk by Prof. Timo Saksala from the Tempre University of Technology, Finland (Numerical modeling of rock fracture using polygonal final elements), a talk by Dr. Elad Priel from the SCE, Israel (A computational study of molybdenum equal channel angular pressing validated by experiments), and the presentation by Dr. Yaniv Brick, a young EE faculty member at Ben-Gurion University, was elected as the best presentation at ISCM-44, titled "Fast low rank approximation of oscillatory kernel integral equation-based off-diagonal matrix blocks ". *Figure 5* shows Dr. Brick during his talk and *Figure 6*

Figure 6:
IACMM executive council, the international speaker, organizers and some of the speakers at ISCM-44, at the Ben-Gurion University. Left to Right: P. Bar-Yoseph, M. Engelman, Z. Yosibash, S. Krylov, D. Givoli, S. Hartmann, P. Trapper, Y. Feldman, I. Harari, A. Herszage, Y. Brick and E. Gal

is a group photo of the Invited speaker with the IACMM executive council and some of the speakers at ISCM-44.

The first prize winner of the best presentation at ISCMs in 2017, Ms. Dana Bishara, and the second prize winner, Ms. Hanan Amar, received an IACMM certificate awarded by IACMM president Prof. Zohar Yosibash during the assembly meeting of IACMM held at ISCM-44. *Figure 7* shows Ms. Bishara and Prof. Yosibash during the awarding ceremony. Being the first prize winner, Ms. Bashara was awarded a financial support by the IACMM to present her talk at the WCCM 2018 conference held in July 2018 in New-York. ●

Figure 7:
Ms. Dana Bishara receiving the certificate on best presentation in 2017 from Prof. Yosibash (president of IACMM) during the General Assembly of the IACMM at ISCM-44

4th Association of Computational Mechanics Taiwan (ACMT) Conference

4th ACMT Conference Organizing Committee:

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The Association of Computational Mechanics Taiwan (ACMT) was founded in 2007 to strengthen the development and collaboration between researchers in the field of computational mechanics in Taiwan. Many members of ACMT are also regular minisymposium organizers and speakers for WCCM and APCOM events. Starting from 2015, ACMT holds an annual meeting on October to furthermore promote the field of computational mechanics in Taiwan. The fourth conference of the association was a joint conference held in Yilan, Taiwan in conjunction with the second International Conference on Mechanics, the 12th Asian Computational Fluid Dynamics Conference, 25th National Computational Fluid Dynamics Conference during **October 15-18, 2018**. The event attracted more than 250 participants from universities, research institutes and industries. In addition to domestic participants from Taiwan, plenary, semi-plenary, keynote speakers and participants from USA, UK, Japan, China, Korea etc. attended the conference.

Figure 1:
Opening by Prof. Chao-An Lin

Figure 2:
Plenary speech by Prof. Yue Yang

Figure 3:
Plenary speech by Dr. Chen-Tang Wu

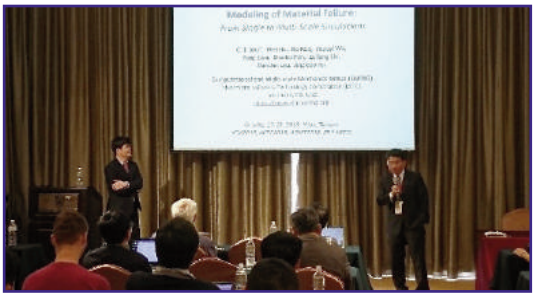

Figure 4:
Plenary speech by Prof. Eckart Meiburg

The ACMT conference emphasizes on the synthesis of computational solid mechanics and computational fluid mechanics communities in Taiwan. This year it featured 9 plenary speeches, 2 from computational solid mechanics and 7 from computational fluid mechanics. The plenary speeches were given by Prof. Michael Leschziner (Imperial College) on influence of outer large-scale structures on wall friction, Prof. Yue Yang (Peking University) on evolution of vortex-surface fields, Dr. Chen-Tang Wu (LTSC) on computational modeling of materials failure, Prof. Eckart Meiburg (University of California, Santa Barbara) on double-diffusive sedimentation, Prof. Kawnjung Yee (Seoul National University) on numerical simulation for aircraft icing, Pro. Gour-Tsyh Yeh (National Central University) on CFD with MMOC approaches, Prof. Makoto Tsubokura (Kobe University) on unified simulation framework for continuum mechanics, Prof. Jyh-Chen Chen (National Central University) on numerical simulative application on silicon crystal growth, and Prof. Kuo-Ning Chiang (National Tsing Hua University) on failure life prediction with AI technology, respectively.

The conference also featured 6 session keynote lectures, 13 invited symposia, 163 oral presentations and 28 posters. There were 20 sessions for topics of methods and applications related to various aspects of computational mechanics and interdisciplinary topics, including, bio-medical applications, materials modeling, fluid-structure interaction, materials genome, etc. We also took this opportunity to host ACMT executive council and general council meetings. All the members are very excited about the growth prospect of the association.

The 4th ACMT Conference was a great success. We appreciate the support of plenary and semi-plenary speakers, keynote speakers, the minisymposia organizers and strong involvement of the participants.

The 5th ACMT Conference will be held in conjunction with the **7th Asia-Pacific Congress on Computational Mechanics (APCOM)** on **December 18-21, 2019**. We look forward to the coming event and opportunities to give impetus for a strong computational mechanics community in Taiwan. ●

Figure 5, 6 and 7:
ACMT Executive and General Council Meetings

conference diary planner

17 - 18 Jan 2019	**Uncertainty Quantification in Computational Solid and Structural Materials Modeling**		
	Venue: Baltimore, Maryland	*Contact:*	http://uq-materials2019.usacm.org
31 Mar. - 3 Apr. 2019	**FEF-2019 - Finite Elements in Fluids**		
	Venue: Chicago, IL	*Contact:*	http://www.fef2019.org/
10 - 12 April 2019	**UKACM2019 - UK Association for Computational Mechanics**		
	Venue: London, UK	*Contact:*	http://ukacm.org/
13 - 15 May 2019	**MARINE 2019 - VIII International Conference on Computational Methods in Marine Engineering**		
	Venue: Gothenburg, Sweden	*Contact:*	http://congress.cimne.com/marine2019/
22 - 24 May 2019	**IPM 2019 - 5th Int.l Conference on Inverse Problems in Mechanics of Structures & Materials**		
	Venue: Rzeszow, Poland	*Contact:*	https://ipm.prz.edu.pl/
27 - 29 May 2019	**ADMOS VIII - International Conference on Adaptive Modeling and Simulation**		
	Venue: Campello (Alicante), Spain	*Contact:*	http://congress.cimne.com/admos2019/
3 - 5 June 2019	**COUPLED PROBLEMS -VIII Int. Conference on Coupled Problems in Science & Engineering**		
	Venue: Barcelona, Spain	*Contact:*	http://congress.cimne.com/coupled2019/
10 - 12 June 2019	**6th International Conference on Computational and Mathematical Biomedical Engineering**		
	Venue: Sendai City, Japan	*Contact:*	http://www.compbiomed.net/2019/
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/
1 - 3 July 2019	**CMN 2019 - Congreso de Métodos Numéricos en Ingeniería**		
	Venue: Guimarães, Portugal	*Contact:*	http://www.cmn2019.pt/index.php/pt/
1 - 3 July 2019	**M-FET 2019 - 2nd Modern Finite Element Technologies - Mathematical & Mechanical Aspects**		
	Venue: Bad Honnef, Germany	*Contact:*	http://mfet2019.de/
15 - 18 July 2019	**MULTIBODY 2019 - Multibody Dynamics**		
	Venue: Duisburg, Germany	*Contact:*	https://www.uni-due.de/eccomasmultibody2019/
28 Jul. - 1 Aug. 2018	**USNCCM 15 - 15th US National Congress on Computational Mechanics**		
	Venue: Austin, TX	*Contact:*	http://15.usnccm.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/
11 - 13 Sept. 2019	**Sim-AM 2019 - II International Conference on Simulation for Additive Manufacturing**		
	Venue: Pavia, Italia	*Contact:*	http://congress.cimne.com/sim-am2019/
12 - 14 Sept. 2019	**EUROGEN 2019 - Int. Conf. on Evolutionary & Deterministic Methods for Design, Optimization & Control**		
	Venue: Guimarães, Portugal	*Contact:*	http://eurogen2019.dep.uminho.pt/
18 - 20 Sept. 2019	**IGA 2019 - VI International Conference on Isogeometric Analysis**		
	Venue: Munich, Germany	*Contact:*	http://congress.cimne.com/IGA2019/
18 - 20 Sept. 2019	**COMPOSITES 2019 - VII Conference on Mechanical Response of Composites**		
	Venue: Girona, Spain	*Contact:*	http://composites2019.udg.edu/
7 - 10 Oct. 2019	**Form & Force - joint 60th IASS Symposium 2019 & 8th Structural Membranes 2019**		
	Venue: Barcelona, Spain	*Contact:*	http://congress.cimne.com/Formandforce2019/
16 - 18 Oct. 2019	**3rd Int. Conf. on Recent Advances in Nonlinear Design, Resilience & Rehabilitation of Structures**		
	Venue: Coimbra, Portugal	*Contact:*	https://corass2019.dec.uc.pt/
28 - 30 Oct. 2019	**PARTICLES 2019 - VI International Conference on Particle-Based Methods**		
	Venue: Barcelona, Spain	*Contact:*	http://congress.cimne.com/particles2019/
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/