CHARACTERIZING YOUNG'S MODULUS OF GRAPHENE/EPOXY NANOCOMPOSITES USING MULTISCALE SIMULATION

Jia-Lin Tsai, Tai-Yuan Wang, Po-Ying Tseng

[1 2 3]*Department of Mechanical Engineering, National Chiao Tung University, Hsinchu, Taiwan*

Atomistic simulation together with micromechanical analysis was employed to model the Young's modulus of graphene/epoxy nanocomposites. The nanocomposites containing pristine graphene, carboxyl (COOH)-functionalized graphene, and COOH- and amine (NH_2)-functionalized graphene were considered in the simulation. In order to characterize the mechanical behaviors of graphene/epoxy nanocomposites, an ideal atomistic nanocomposite model was constructed. Based on the molecular dynamic simulation, the moduli of the atomistic nanocomposites were then evaluated from uniaxial tensile loading. Through the equivalence of the deformed energy in the atomistic model and continuum finite element model, the effective properties of a continuum graphene in the nanocomposites were derived. The effect of atomistic interaction between atomistic graphene and the surrounding epoxy was embedded in the effective properties of the graphene. Subsequently, the Young's moduli of nanocomposites with randomly oriented graphene were modeled from the Mori–Tanaka micromechanical model. The results indicated that the COOH- and NH_2-functionalized graphene nanocomposite exhibited superior mechanical properties to those of the other two material systems. Moreover, the model predictions were in good agreement with the experimental data.

Keywords: Multiscale modeling; Young's modulus; Graphene/epoxy nanocomposites

DEGREE OF IRREGULARITY OF MICROSTRUCTURE IN UNIDIRECTIONAL COMPOSITES AND ITS INFLUENCE ON ANISOTROPY OF ELASTIC PROPERTIES

Robert Zemčík[1,*], Hana Srbová[2], Tomáš Kroupa[3]

[1] NTIS – New Technologies for Information Society, Faculty of Applied Sciences, University of West Bohemia in Pilsen, Univerzitní 8, 30100 Plzeň, Czech Republic, zemcik@kme.zcu.cz

[2] NTIS – New Technologies for Information Society, Faculty of Applied Sciences, University of West Bohemia in Pilsen, Univerzitní 8, 30100 Plzeň, Czech Republic, hsrbova@kme.zcu.cz

[3] NTIS – New Technologies for Information Society, Faculty of Applied Sciences, University of West Bohemia in Pilsen, Univerzitní 8, 30100 Plzeň, Czech Republic, kroupa@kme.zcu.cz

The layers of unidirectional (UD) continuous fiber-reinforced composites (FRC) are usually considered to be transversely isotropic material. The approach is based on the assumption that the fibers are distributed regularly in perfect hexagonal pattern in the plane transverse to fiber direction and that all fibers have the same cylindrical shape and diameter. However, both the distribution and fiber shape in real material samples are always irregular, which can lead to significant difference in the predicted elasticity properties when using either analytical approaches, such as simple rule of mixtures or homogenization techniques, or numerical approaches using periodical unit cell models. The only parameter that plays role in this analysis in case of the regular distribution is the fiber volume content (or ratio).

Therefore, a new parameter Υ is proposed in this work to describe the degree of irregularity (DOI) of the spatial distribution in the composite transverse plane (cross-section). It is calculated on a representative volume element (RVE), representing either periodical or non-periodical unit cell of the material structure. The value of this parameter is influenced by variation of fiber diameters, misplaced fiber positions, missing or additional fibers, and it is rotation independent. It is defined as sum over all fibers in RVE of squared differences between areas of intersection (AOI) of group of fibers between irregular and regular distributions normalized by cell dimensions (size).

Various random geometries of periodical unit cell (PUC) having different distribution of fibers but keeping the same FVC are generated using pseudo-physics algorithm resembling the motion of magnetic particles. The geometries are based on SEM (scanning electron microscopy, see Fig. 1) images of various materials. Several special geometries are designed manually in order to achieve the extreme unnatural irregularity, hence extreme values of the new DOI parameter Υ, such as compact cluster or compact stripe of closely packed fibers (see Fig. 2) or various geometries with holes (i.e. missing fibers) in the regular distribution.

Finite element models of the generated structures we created using Python scripts in Abaqus 6.14. The models are prepared so that exact periodical boundary conditions can be applied. The homogenized (or effective) elastic properties (engineering constants E, ν and G) are obtained from six uniaxial tests and their extremal values are sought by rotation of coordinate system about x axis within the transverse cross-section (yz plane). The results are compared with the constant values in the isotropic case (regular PUC) and they are correlated with the DOI parameter.

The results show significant dependence on the proposed DOI parameter since the elastic properties show increasing variation with increasing value of ϒ (see Fig. 2). The DOI parameter could be used for the quantitative representation of quality of real material structure and for the prediction of its heterogeneity and anisotropy.

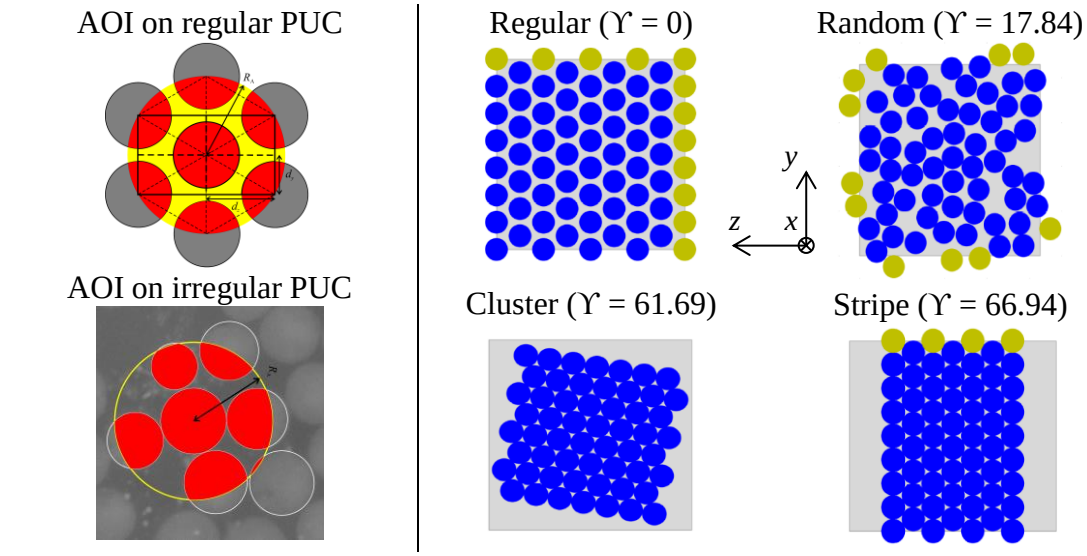


Figure 1 LEFT: Scheme of definition of area of intersection (red color) used in the calculation of DOI parameter (top – regular distribution, bottom – real distribution in SEM image). RIGHT: Geometries of PUCs in *yz* plane having the same FVC (regular, cluster, stripe and random). Yellow circles represent periodically mirrored fibers.

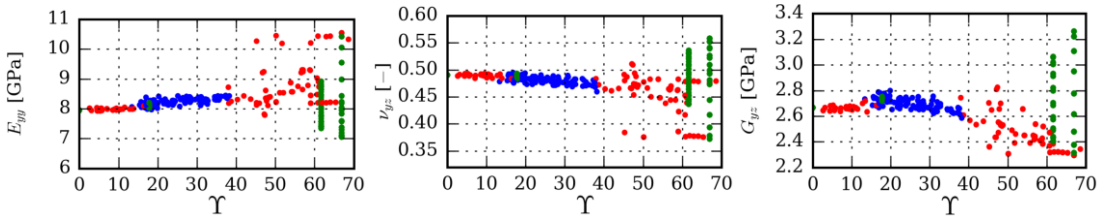


Figure 2 Influence of DOI parameter on the variation of selected elasticity properties. Vertical groups of green dots correspond to the PUCs in Fig. 1 (rotated about *x* axis by 5° steps – see the ϒ values). Red and blue dots represent additional random PUCs (different settings of proposed algorithm).

Acknowledgement

This publication was supported by the project LO1506 of the Czech Ministry of Education, Youth and Sports.

References

[1] Nemeth, M.P. An In-Depth Tutorial on Constitutive Equations for Elastic Anisotropic Materials, NASA/TM–2011-217314 report, Langley Research Center, 2011.

[2] Christensen, R.M. Sufficient Symmetry Conditions for Isotropy of the Elastic Moduli Tensor. Journal of Applied Mechanics, 54:772–777, 1987. DOI: 10.1115/1.3173115.

[3] Yang, J. Development about composite homogenization in static and in dynamic – application to UD composite materials. Master's thesis, Ecole Centrale de Nantes, Nantes.

MULTI-SCALE MODELLING OF THE UNSATURATED-SATURATED FLOW IN A SHALLOW AQUIFER SYSTEM

Jicai Zeng, Yuanyuan Zha, Jinzhong Yang*

Address: No. 8th Donghu South Road, Wuhan 430072, PR China

e-mail: {jczeng, zhayuan87, jzyang}@whu.edu.cn

ABSTRACT

For subsurface flow simulation within a shallow aquifer system, the vertical interactions between the soil water and the underlying groundwater body are usually intensive. To better understand the unsaturated-saturated flow processes in this context, the soil physicists obtain an arduous solution by solving the Richards' equation at small scale, while the geologists take advantage of the easily-solved groundwater equation for an ambiguous solution of the groundwater flow at large scale. These single-scale models therefore fail to depict the water-flow details in a regional-scale shallow aquifer even using very fine grids and time steps due to the controversy of accuracy and computational burden. In this presentation, a multi-scale model for simulating the large-scale saturated groundwater flow and small-scale variably saturated flow is proposed. The multi-scale issue in this work lies in 1) the scale-separation methodology for the complicated flow simulation at different scales and 2) the mutual compensation of head and flux boundaries for models at different scales with a two-way coupling scheme. For variably saturated flow models at small scale, the time-varying boundaries around and below the subdomains have to be delivered downward from the large-scale groundwater model. A three-dimensional Darcy-based interpolation method[1-2] is utilized to achieve this by generating spatially and temporally refined head boundaries for small-scale models. For groundwater model at large scale, the upper boundary, which overlaps the lower boundary of the soil-water flow, has to be derived from the independently discretized small-scale variably-saturated flow models. During each large-scale time step, an empirical equation for determining the overall upper boundary of the large-scale model is updated with a multiple linear regression model. The regression model is devoted to link the small-scale solution, i.e., the instant recharge rate at the water table, with the large-scale information, such as soil texture, precipitation, irrigation, evapotranspiration, and water-table fluctuation. The proposed multi-scale model is validated with two test cases for investigating the performance of the regression model and the efficiency of the two-way coupling scheme.

Key words: multi-scale modelling; unsaturated-saturated flow simulation; multiple linear regression model; shallow aquifer; two-way coupling

References

[1] Jicai Zeng, Yuanyuan Zha, Liangsheng Shi, Yan Zhu, Jinzhong Yang*, 2017. On the sub-model errors of a generalized one-way coupling scheme for linking models at different scales, Advances in Water Resources. Revision Requested.

[2] Jicai Zeng, Yuanyuan Zha, Jinzhong Yang*, 2017. A Coupling Model for Multi-scale Flow Simulation in a Large Scale Groundwater System, Journal of Hydraulic Engineering. Revision Requested.

REDUCED ORDER FUZZY-STOCHASTIC FEM BASED HOMOGENIZATION FRAMEWORK FOR HETEROGENEOUS MATERIALS WITH POLYMORPHIC UNCERTAINTIES IN THE MICROSTRUCTURE

Dmytro Pivovarov [1,*], Thomas Oberleiter[1], Kai Willner[1], Paul Steinmann[1]

[1] Chair of Applied Mechanics, Friedrich-Alexander University Erlangen-Nürnberg,
Egerlandstraße 5, 91058 Erlangen, Germany
E-mail: dmytro.pivovarov@fau.de

In the present study we perform computational homogenization of heterogeneous materials. Due to geometrical uncertainties in the microstructure non-deterministic homogenization techniques are required. Based on the analysis of experimental data two different sources of uncertainties are considered – aleatoric, which result from the natural variability of the microstructure and they can be described in terms of a probability density, and epistemic, which results from our lack of knowledge about the microstructure and also require other simulation techniques like, e.g., fuzzy arithmetic. Combination of both types of uncertainties is referred to as polymorphic, which is typical for real materials. Thus in the present work we establish the conjunction of the earlier proposed stochastic FEM with local description of the stochastic space [1, 2] and fuzzy arithmetic techniques. Due to the fact that both approaches are computationally expensive, order reduction techniques are discussed. Convergence and accuracy of reduced order models are studied, wherein the full order model and Monte-Carlo simulations are used as reference solution.

References

[1] Pivovarov D., Steinmann P., 2016. Modified SFEM for computational homogenization of heterogeneous materials with microstructural geometric uncertainties. Computational Mechanics 57, (1), 123–147.

[2] Pivovarov D., Steinmann P., 2016. On stochastic FEM based computational homogenization of magneto-active heterogeneous materials with random microstructure. Computational Mechanics, 58(6), 981–1002

MULTI-SCALE COMPUTATIONAL MODELING FOR CONCRETE DAMAGE CAUSED BY MIXED PORE PRESSURES FROM COUPLED ALKALI SILICA REACTION AND FREEZE/THAW CYCLES

Fuyuan Gong[1,*], Yuya Takahashi[2], Koichi Maekawa[3]

[1]Department of Civil Engineering, The University of Tokyo, gong@concrete.t.u-tokyo.ac.jp

[2] Department of Civil Engineering, The University of Tokyo, takahashi@concrete.t.u-tokyo.ac.jp

[3] Department of Civil Engineering, The University of Tokyo, maekawa@concrete.t.u-tokyo.ac.jp

As one kind of porous media, concrete suffers from many kinds of ambient impacts which can be owned to the arising pore pressures. Freeze/thaw cycles (FTC) and alkali silica reaction (ASR) are such two typical impacts that may happen together, and cause mixed expansive pressure in micro-pores but finally result in macroscopic damage to concrete structures. In order to investigate the macro-mechanical behaivor of concrete material affected by the micro-events, a multi-scale compulationational model is developed based on the FEM computation program DuCOM-COM3D in this study, the analysis system covers from the hydration of cement paste and finally to the mechacnical performance of bulk concrete.

The micro-physical events are computationally modeled considering the coupling effect between ASR gel and water in the mixed pressure and motion. The pressures and transportation of pore substances are also linked with the concrete matrix deformation at macroscale through a poromechanical approach, and will affect with each other reciprocally. Once the crack happens in the nonlinear analysis, both the micro-events (water and gel motion) and the macro mecahnical behavior will be affacted. Finally, different sequences of combined ASR and FTC are simulated. The computation program can quantatitively reproduce the physical events in pore structures, and further the macro-damages. The results show that ASR can reduce the FTC expansion for non-air-entrained concrete but increase the frost damage for air-entrained concrete.The simulated behaviors also agree well with the previous experimental phenomena.

AN EFFICIENT SHALLOW WATER HYDRO-SEDIMENT-MORPHYDYNAMIC MODEL FOR ALLUVIAL RIVERS

Peng Hu[1], Jianjian Han[2], Zhixian Cao[3], Huaihan Liu[4], Zhiguo He[5], Zhiyuan Yue[6]

[1] Ocean College, Zhejiang University, Hangzhou, China. Email: pengphu@zju.edu.cn

[2] Ocean College, Zhejiang University, Hangzhou, China. Email: 572146662@qq.com

[3] State Key Laboratory of Water Resources and Hydropower Engineering Science, Wuhan University, China. Email: zxcao@whu.edu.cn

[4] Changjiang Waterway Bureau, Wuhan, China. Email: 516930205@qq.com

[5] Ocean College, Zhejiang University, Hangzhou, China. Email: hezhiguo@zju.edu.cn

[6] Changjiang Institute of Survey, Planning, Design and Research, Wuhan, China. Email: yuezhiyuan1982@126.com

Motivation: Numerical integration of the shallow water equations using finite volume Godunov-type shock-capturing schemes has become increasingly popular due to its advantages in dealing with complex flow regimes and wet/dry fronts etc. Under this modeling framework, inclusion of sediment transport and bed deformation is straightforward, which apparently involve multi-scale and multi-physical processes. The last several decades have witnesssed wide applications of shallow water hydro-sediment-morphydynamic models (Cao *et al*. 2017). However, this type of models are computationally demaining (Sanders 2008; Dazzi *et al*. 2016), especially when large-scale and long-duration events are to be resolved. This is in particular the case when local flow effects must be taken into account, which necessitates locally refined meshes. Here we present a 2D shallow water hydro-sediment-morphydynamic model, in which local-time-stepping (LTS) is implemented, and assess its potential for saving the computational time for engineering applications.

Hydro-sediment-morphydynamic model: The complete depth-averaged governing equations are solved by the finite volume method on unstructured mesh. The HLLC approximate Riemann solver is used to estimate the numerical fluxes across the face between neighboring cells. The bed deformation and sediment compositions are updated at the cell center. The bed slope is estimated using bed elevations defined at the cell nodes. This model was originally developed using the global time step (GTS) Δt_g that is the same throughout the computational domain. It has been validated against classical data set, including dam-break flow, bed aggradation and degradation cases.

Local time step (LTS): A LTS scheme has been proposed by Sanders (2008) and modified by Dazzi *et al*. (2016) for modeling clear-water flows. Here it is implemented in the above hydro-sediment-morphodynamic model. First, the LTS Δt_i in cell-*i* is set as m_i power of two multiple of the global time step Δt_g. The exponent m_i takes the largest interger that ensures satisfaction of the local CFL condition and at the same time must not exceed a pre-defiend value m_a, which is referred to the LTS-level. The LTS level determines the difference between the smallest and largest time step. To complete an update of all cells, the model carries out a LTS Δt_i cycle of 2^{ma} time loops. At each LTS loop, numerical fluxes and source terms are estimated only for cells that requrie updating. The LTS is implemented only for the equations that have advection terms, whereas for bed deformation and sediment compostions, the largest time step is used.

Case study - the middle Yangtze River: In the past ten years, conflict between the bridge safety and navigation becomes more and more intense for the Taipingkou waterway (an anabranching reach of about 20 km long and 2.0 km wide in the Middle

Yangtze River). While the north branch experiences intense sediment deposition and thus has a high risk for shiping during low water, the bridge piers in the south branch are vulunable to ship collisions. Formulating futher regulating schemes requires enhanced understanding on the morphological evolutions of the central bar and the two branches, for which the flow structures around the piers must be numerically resolved. Since the horizontal length scales of the piers are about 4 m, one has to resort to locally refined meshes (Fig. 1a), which leads to a GTS of about 0.05-0.08 s, as indicated by the minimum value of the lcoal time step in Fig.1b. Estimates indicate that using the GTS requires a running time of about six month for a one-year simulation for this reach. In contrast, using LTS-level 5, the running time of the present model is reduced to about two weeks, corresponding to a reduction of about 90% in the running time. This reduction is significant for systematic investigation of the morphological evolution of this reach. As shown in Fig. 2, the computed bed deformation for a one-year period (2003-2004) indicates erosion for the south branch and deposition in the north branch. Further numerical case studies are ongoing, aiming to reveal effects of different factors on the morphological evolution of this reach.

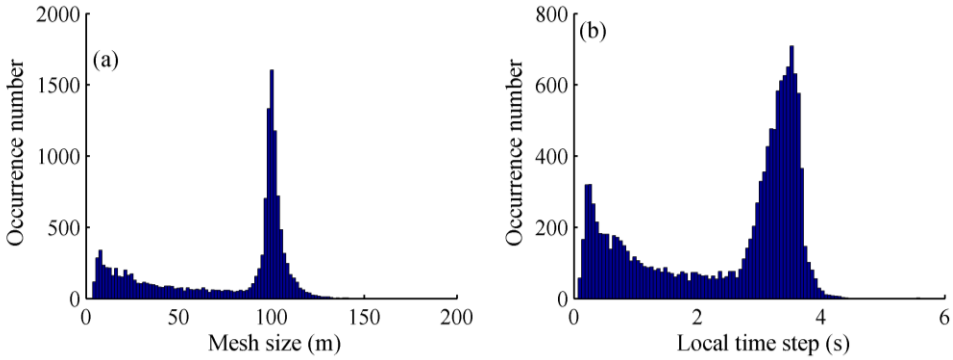


Figure 1 Occurrence number of cells for (a) mesh sizes, and (b) local time step for the Taipingkou waterway

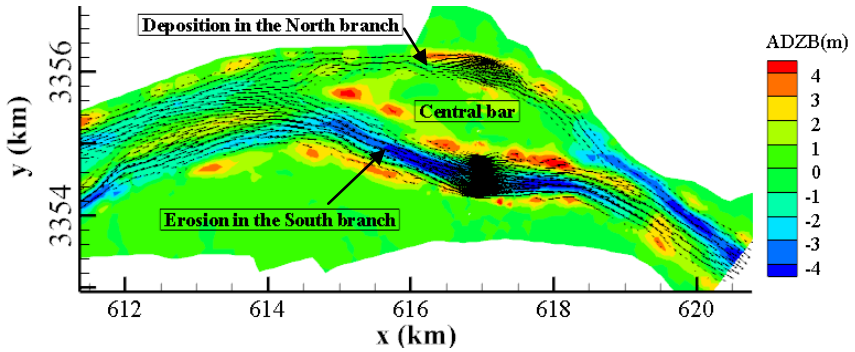


Figure 2 Computed bed deformation depth (ADZB) from March 2003 to March 2004

References

[1] Cao, Z., Xia, C., Pender, G., and Liu, Q. 2017. Shallow water hydro-sediment-morphodynamic equations for fluvial processes. *Journal of Hydraulic Engineering* ASCE, DOI: 10.1061/(ASCE)HY.1943-7900.0001281, in press.

[2] Dazzi, S., Maranzoni, A., and Mignosa, P. 2016. Local time stepping applied to mixed flow modeling. *Journal of Hydraulic Research* 54, 145-157.

[3] Sanders, B. F. 2008. Integration of a shallow water model with a local time step. *Journal of Hydraulic Research* 46, 466-475.

A probability transformation method (PTM) for the dynamic stochastic response of structures with non-Gaussian excitations

Giovanni Falsone, Rossella Laudani

Dipartimento di Ingegneria, Università di Messina, C.da Di Dio, 98166 Messina - Italy
gfalsone@ingegneria.unime.it, rossellalaudani@hotmail.it

The random characterization of the response of a structural time-dependent system often requires a high computational effort, above all when the response is a non-Gaussian process. Actually, even for a system subjected to static non-Gaussian actions, the computational effort can be very high; this is essentially due to the high number of random variables, usually not independent, defining the response involved. Moreover, for the non-Gaussian response processes, the characterization is made through the evaluation of the corresponding statistical moments or the cumulants, and this increases considerably the problem dimensions, without reaching the complete characterization of the response. Indeed, the full probabilistic characterization of a random variable is given by the knowledge of its probability density function, or by its characteristic function. Unfortunately, in the literature a few of methods exist working directly on the response probability density functions, without passing through the moments or the cumulants. The only exception is when both the input and the output are Gaussian.

Even for the dynamics systems, the evaluation of the random response is often limited to the evaluation of the second order correlations, or power spectral densities if the analysis is performed in the frequency analysis. In any case, no paper has been found in the literature based on the direct relation between the probability density function of the time-dependent input and that one of the time-dependent output. The benefit of an approach of this type appears to be even more evident in the dynamical case.

Aim of this work is to show an approach able to give instant by instant a direct relation between the two probability density functions of input and output of a linear system. This approach represents an extension of the Probabilistic Transformation Method (PTM), introduced by Falsone and Settineri, first for the static problem [1], and then for a first attempt in the dynamical case [2]. In particular, in this work, some drawbacks highlighted in [2] are overcome, arriving to an effective approach, for both accuracy and computational effort.

References

1. G. Falsone, D. Settineri, Explicit solutions for the response probability density function of linear systems subjected to random static loads**,** *Probabilistic Engineering Mechanics*, vol. 33, 2013, pp.86-94.
2. D. Settineri, G. Falsone, A method for the evaluation of the response probability density function of some linear dynamic systems subjected to non-Gaussian random load, *Probabilistic Engineering Mechanics*, **38**, 2015, 165–172.

MODEL ORDER REDUCTION IN NONLINEAR ELASTIC FULL WAVEFORM INVERSION BY DECOMPOSING THE MODEL SPACE

Vladimir Tcheverda[1,*], Kirill Gadylshin[2], Guy Chavent[3]

[1]Institute of Petroleum Geology and Geophysics, e-mail: vova_chev@mail.ru

[2]Gadylshin Kirill, Institute of Petroleum Geology and Geophysics, e-mail: gadylshinkg@ipgg.sbras.ru

[3]Guy Chavent, INRIA, e-mail: guy.chavent@inria.fr

Full Waveform Inversion (FWI) combines a group of methods based on nonlinear least squares approach to solve dynamic inverse problem of waves' propagation. This problem consists in solving the nonlinear operator equation $F(m) = d$ with operator $F: M \to D$ which acts from the model space M (waves propagation velocity) to the data space D (seismic data acquired at some points on the surface $z=0$). The action of this operator to some current model is given as a solution to the boundary-value problem for Helmholtz equation

$$\Delta u + \frac{\omega^2}{m(x,z)} = G(\omega)\delta(x - x_s, z - z_s)$$

with subsequent projection of the solution to reciever positions.

Standard approach to search for $m(x,z)$ is nonlinear least square minimization of the data misfit functional which characterizes $\boldsymbol{L_2}$ residual between observed and synthetized data for a current velocity model:

$$m_* = argminE(m), \qquad with\, E(m) = ||F(m) - f||_D^2$$

This approach has been developed and studied in a great number of publications (see (Virieux and Operto, 2009), and the references therein), but up to now there are problems with reliable reconstruction of macrovelocity (propagator) component with realistic frequency bandwidth and offsets of the data. Here is necessary to explain that there are two main constituents of the velocity model:

a) Macrovelocity or propagator – is described by smooth functions and, hence, does not return propagation of the seismic energy to the acquisition, but governs the travel time between two remote points inside the medium;
b) Reflectors – local variations of parameters, which do not violate propagation time of the seismic energy, but change returns this energy to the acquisition.

Intuitively this trouble can be explained by the so-called "cycle- skip" effect when phase shifts of the observed and synthetic data may result in local minima. To mitigate the problem, in the papers (Bunks et al., 1995; Pratt et al., 1998) was introduced a multiscale inversion strategy when the frequency of the input data increased progressively and the inversion result for lower frequency becomes an initial guess for the higher frequency. However, such sequential inversion approach also fails due to lack of low frequencies in the data (Sirgue, 2006).

We propose the alternative to this standard formulation. The key stone of this alternative is modification of the data misfit functional on the bast of the model space decomposition into two subspaces:

- subspace of smooth propagators p (macro velocity components);
- subspace of spatial reflectors r.

Moreover, we rely on the common knowledge that reconstruction of reflectors for known propagator is "easy" problem and can be resolved by application of the so-called migration procedure to the data. This procedure actually is the first iteration of minimization process by some gradient-like technique. On this base, we decompose the full model as

$$m = p + r = p + WM(p) < s >,$$

where p is the propagator, s is the "*time reflector*", M – migration operator, W weighted matrix, equalizing amplitudes of spatial reflectors.

Now we modify the data misfit functional as

$$E(p, s) = ||F(p + WM(p) < s >) - d||_D^2,$$

and do minimization within the model space by turn with respect to the propagator and time reflector. As one can see minimization with respect to time reflector s is really "easy" as it enters linearly in the argument of the forward map. At the same time, dependence on the propagator is essentially nonlinear and very complicated. Fortunately, subspace of propagators has very low dimension as it is made of smooth functions, while reflectors are high oscillating and, hence, form high-dimensional subspace.

We validate this approach by reconstruction of the famous Marmoussi model (Fig.1). Acquisition has 9000 meters of lengthб 460 receivers and 46 volumetric sources spaced with 20 and 200 meters respectively. Frequency range is 5 – 15 Hz. We search propagator from the subspace spanned on 20 cubic B-splines.

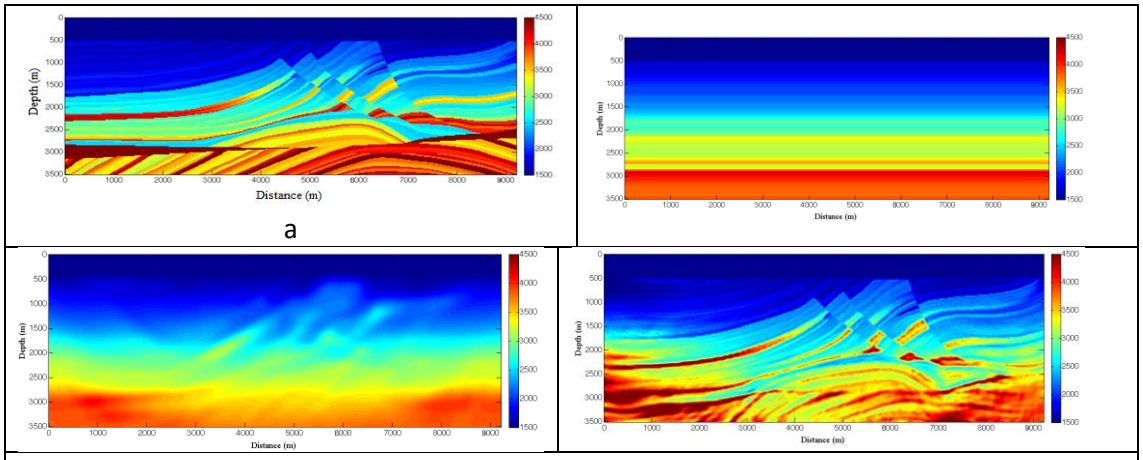


Figure 1. a) *Exact Marmoussi model b) Initial guess for inversion; c) reconstructed macrovelocity/propagator; d) reconstructed full Marmoussi model (propagator+reflector)*

References

[1] Virieux, J., Operto, S. [2009] An overview of full-waveform inversion in exploration geophysics. *Geophysics*, **74**(6), WCC1-WCC26.

[2] Bunks, C., Saleck, F.M., Zaleski, S. and Chavent, G. [1995] Multiscale seismic inversion.

Geophysics, **60**(05), 1457-1473.

[3] Pratt, G., Shin, C., Hicks, G.J. [1998] Gauss-Newton and full Newton methods in frequency space seismic waveform inversion. *Geophysical Journal International*, **133**(2), 341-362.

[4] Sirgue, L. [2006] The importance of low frequencies and large offset in waveform inversion. *68th EAGE Technical conference and Exhibition*, A037.

CHARACTERISATION OF SPATIAL VARIABILITY IN LATTICE MODELS

Marco Marcon[1], Jan Podrouzek[2,*], Jan Vorel[3], Roman Wan-Wendner[4]

[1] Christian Doppler Laboratory, University BOKU, Vienna, marco.marcon@boku.ac.at

[2] Faculty of Civil Engineering, Brno University of Technology and Christian Doppler Laboratory, University BOKU, Vienna, podrouzek.j@fce.vutbr.cz

[3] Christian Doppler Laboratory, University BOKU, Vienna, jan.vorel@boku.ac.at

[4] Christian Doppler Laboratory, University BOKU, Vienna, roman.wendner@boku.ac.at

Recent developments in particle placement schemes, such as those derived from governing random or gradient based field [1], in the context of the lattice discrete particle modelling (LDPM) [2], have opened the door for new approaches of investigating the spatial variability of heterogenous materials owing to microstructural features. In this paper, the gradient-based fields and random fields are introduced into the stochastic framework of LDPM to account for inherent variability and production process of several concrete specimen test series (fig.1), such as cylinder compression test and three point bending test. As a consequence, the lattice models become sensitive to a particular particle placement concept, which is no longer independent and random [3], and the scattering of the response can thus be associated with the physical meaning of an auto-correlation length and particular forms of the spectral function. Moreover, particular placement concepts, such as the gradient based fields, may also affect the mean values of the response (fig.2).

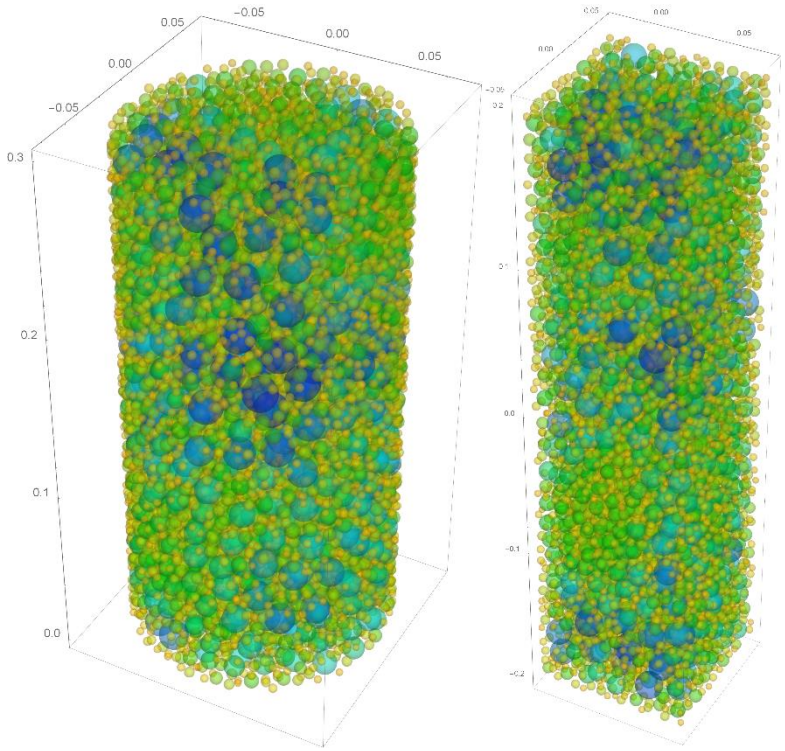


Figure 1: Maximum strength realizations of 2x20 LDPM experiments based on a governing Gaussian random field with a power spectral parameter ($\#^{-2.00}$) maximizing the COV of the load capacity.

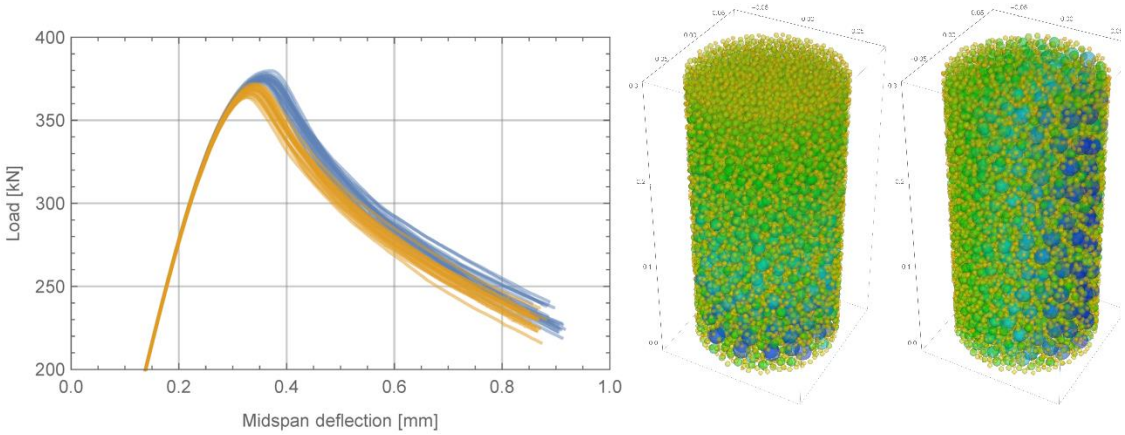


Figure 2: Scattering and shifted L-D diagrams (zoomed-in detail) of LDPM realizations of compression cylinder tests with two gradient-based fields (gravity angle is orange and normal to gravity angle is blue).

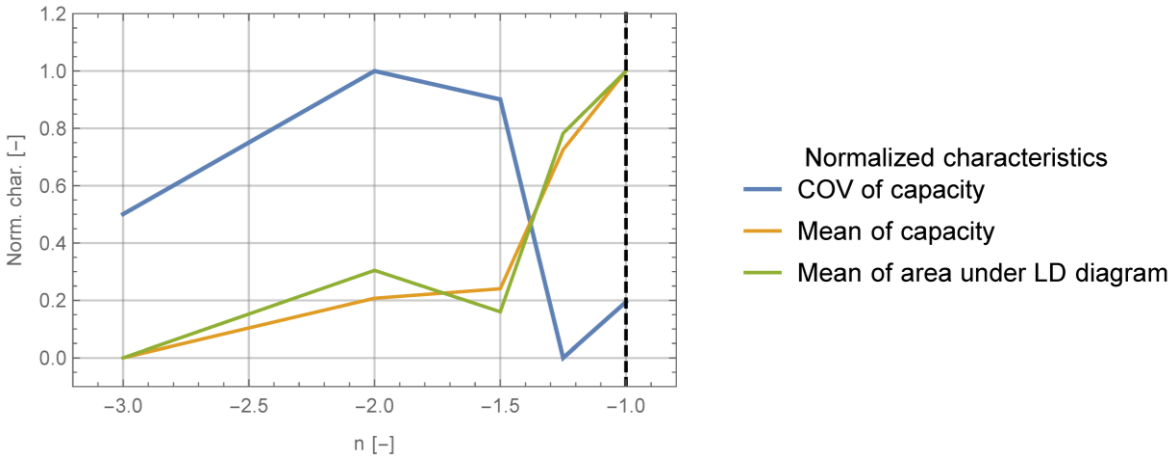


Figure 3: Normalized statistical characteristics vs. power spectral parameter *n*; response of cylindrical compression test series (20 realizations) and Gaussian random field with power spectral function $\#^{-n}$. The dashed line represents the zero correlation reference, i.e. the independent and random placement scheme.

The inverse U-shaped curve for the coefficient of variation of the load capacity (fig. 3) and various power spectral parameters clearly supports the hypotheses on a causal relationship between spatial variability, auto-correlation length of the random fields, type of spectral function and meso/micro-structure of the material. Please note that the material property fields are constant for all presented results.

References

[1] J. Podroužek, J. Vorel, G. Cusatis, and R. Wendner, "Imposed Correlation Between Random Field and Discrete Particle Placement," in *14th International Probabilistic Workshop*, 2016, pp. 245–252.

[2] G. Cusatis, D. Pelessone, and A. Mencarelli, "Lattice Discrete Particle Model (LDPM) for failure behavior of concrete. I: Theory.," *Cem. Concr. Compos.*, vol. 33, no. 9, pp. 881–890, 2011.

[3] J. Podroužek, J. Vorel, I. Boumakis, G. Cusatis, and R. Wendner, "Implications of spatial variability characterization in discrete particle models," in *Proceedings of the 9th International Conference on Fracture Mechanics of Concrete and Concrete Structures*, Berkeley, CA, USA, 2016.

A MULTISCALE MODEL FOR THERMAL CONTACT CONDUCTANCE OF ROUGH SURFACES UNDER LOW APPLIED PRESSURE

O.K. Panagouli, K. Margaronis, V. Tsotoulidou

Laboratory of structural analysis and design, Department of Civil Engineering,

University of Thessaly, Volos, GR-38334, Greece

e-mail: olpanag@uth.gr ; web page: http: http://lsad.civ.uth.gr/

Thermal contact conductance (TCC) plays an important role in heat conduction mechanism when heat flow paths are interrupted. Many studies have been performed to specify the dominant factors of thermal contact conductance in engineering surfaces, which exhibit both microscopic- known as roughness- and macroscopic irregularities arising from waviness. During the last decades it has been recognized that thermal contact conductance (TCC) is a function of several parameters [1-5], where the most important are the type of the contacting materials, the macro- and micro- geometry of contacting interfaces, the temperature of the materials, the interfacial pressure, the lubricant and surface contaminants and the thickness of the interfacial layer. Many studies on thermal contact conductance [6-9] were concentrated on microscopic irregularities by assuming that the macroscopic irregularities of contact are negligible. However, real engineering surfaces aren't perfectly flat, implying that the macroscopic nouniformity can't be ignored, especially in cases where the contact pressure is low. At the microscale, contact occurs through the interaction of surface asperities and these interactions influence the properties of the surfaces at the macroscale. For that, the consideration of lower scales is necessary for the accurate modelling of heat transfer through the contact interfaces.

The aim of this work is to investigate how the asperities of lower scales of contacting surfaces, affect the thermal contact conductance, in interfaces which exhibit both micro and macroscopic irregularities, in the case of small real contact area fraction. For that, in order to take into account irregularities of different scales, the geometry of interfaces is described by fractal interpolation functions. The problem is simplified by considering contact of a rough surface with inelastic behaviour, with a rigid and smooth surface in order to determine the local thermal conductance at real contact points and thus, to take into account phenomena related to lower scales of surface asperities. In the sequence, the macroscopic thermal contact conductance is determined, based on the solution of the problem at the scale of surface asperities. At each scale, both mechanical and thermal portions of the problem are solved by using the F.E. code MSC-MARC. First, the contact nodes are determined by solving the mechanical problem and in the sequence, the thermal conductance at contact nodes is calculated by solving the thermal problem. It must be mentioned here that the code takes into account for the solution of the mechanical problem the changes in the geometry of the interface and in material parameters due to the temperature. Finally, the influence of the interfacial pressure to the local thermal conductance at real contact points and to the macroscopic thermal conductance is investigated, with respect to the different scales of the irregularities of the rough interface and useful conclusions are derived, concerning the role of roughness and waviness on the thermal contact conductance in cases of low contact pressure.

References

[1] Majumdar, A. and Tien, C.L., 1991. Fractal Network Model for Contact Conductance. Journal of Heat Transfer 8, 516-525.
[2] Williamson, M. and Majumdar, A., 1992. Effect of Surface Deformation on Contact Conductance. Journal of Heat Transfer 114, 802-810.
[3] Wolff, E.G., and Schneider, D.A., 1998. Prediction of Thermal Contact Resistance Between Polished Surfaces. International Journal of Heat and Mass Transfer 41, 3469-3482.
[4] Buonanno, G., Giovinco, G. and Massarotti, N., 2003. An Elastoplastic Model of Thermal Contact Conductance Between Nominally Flat Surfaces in Vacuum. International Communication in Heat and Mass Transfer 30, 921-930.
[5] Ciavarella, M., Dibello, S. and Demelio, G., 2008. Conductance of Rough Random Profiles. International Journal of Solids and Structures 45, 879-893.
[6] Cooper, M.G., Mikie, B.B. and Yovanovich M.M., 1969. Thermal Contact Conductance. Int. J. Heat Mass Transfer 12, 279-300.
[7] Mikie, B.B., 1974. Thermal Contact Conductance: Theoretical Consideration. Int. J. Heat Mass Transfer 17, 205-214.
[8] Yuncu, H., 2006. Thermal Contact Conductance of Nominally Flat Surfaces. Heat and Mass Transfer 43, 1-5.
[9] Abuzeida, O.M. and Alnumanb, N., 2013. Thermal Contact Conductance of Elastically Deforming Nominally Flat Surfaces Using Fractal geometry. Industrial Lubrication and Technology 65, 390-398.

FINITE DIFFERENCE SIMULATION OF WAVES' PROPAGATION IN MULTISCALE MEDIA

Galina Reshetova[1,*], Vadim Lisitsa[2], Victor Kostin[3], Vladimir Tcheverda[4]

[1]Institute of Computational Mathematics and Mathematical Geophysics, kgv@nmsf.sscc.ru

[2]Institute of Petroleum Geology and Geophysics, lisitsavv@ipgg.sbras.ru

[3]Institute of Petroleum Geology and Geophysics, kostinvi@ipgg.sbras.ru

[4]Institute of Petroleum Geology and Geophysics, cheverdava@ipgg.sbras.ru

We present a problem-oriented approach, designed for the numerical simulation of seismic wave propagation in models containing geological formations with small-scale heterogeneities. This requires a special treatment increasing the computational complexity of an algorithm in comparison with elastic media without small-scale intrusions. At the same time, such formations are typically relatively small, filling about 25% of the model, thus the local use of computationally expensive approaches can speed-up the simulation essentially. In this paper we discuss both mathematical and numerical aspects of the hybrid algorithm based on local grid refinement paying most attention to its parallel implementation. Essential efforts are spent to couple different finite-difference stencils. The main issue in the coupling is to suppress numerical artifacts down to the acceptable level, usually a few tenth of the percent.

The algorithm is developed to study scattering and diffraction of seismic waves on clusters of small-scale heterogeneities such as fractures, cavities and karstic formations. In realisitic geological media they usually do not describe each singularity (fracture, caves, karstic intrusion) but describe their volumetric distribution. We assume that the reservoir model is given on a sufficiently fine grid, which possesses grid steps of the size of the first tens of centimeters. A typical seismic wave has a wavelength of about several dozen meters, hence for simulation of waves' propagation in the reference medium (without smal scale intrusions) they use the spatial grid with cells about several meters. Thus, a local mesh refinement is used to perform the full waveform simulation of long wave propagation through a reservoir with a fine structure. As explicit finite differences are used, the size of the time step strongly depends on the spatial discretization and so the time stepping should be local. As a result, the problem of simulation of seismic wave propagation in models containing small-scale structures becomes a mathematical problem of the local time-space mesh refinement.

Consider how coarse and fine grids are coupled. The necessary properties of the finite difference method, based on a local grid refinement are stability and an acceptable level of artificial numerical reflections. Normally scattered waves have an amplitude about 1% of the incident wave, thus the amplitude of artifacts should be at most 0.1% of the incident wave. We modify approach proposed in (Collino, Fouqet and Joly, 2003) so that the grid is refined on two different surfaces surrounding the target area with microstructure. Decoupling of the temporal and spatial grid refinements happened to be the key ensuring acceptable level of numerical artefacts.

As one can see in Fig.1 there is necessary to interpolate data when moving from coarse to fine grid. Interpolation in time is straightforward and does not produce any visible artefact. The main attention we pay to interpolation in space. It is implemented on the base of two dimensional Fast Fourier Transform (2D FFT). As known this kind of interpolation possesses exponential accuracy. This is what makes it possible to reduce artifacts and to the required levlel in tenths of percent to the amplitude of the incident wave.

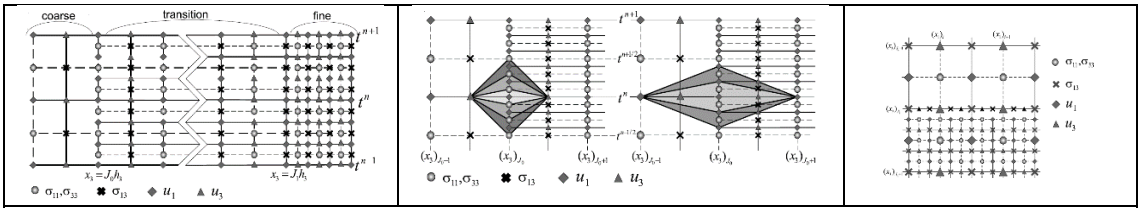


Figure 1. Sketch of grid refinement. Left – transition from coarse-to-fine. Middle – refinement in time. Right – refinement in space.

To validate the approach presented we choose the model with karstic layer (see Fig.2 left). As it is 2D model we are in position to use sufficiently small grid (0.5 meters) to describe small scale heterogeneities in this layer and perform 'exact full-scale' simulation of seismic waves' propgation. The result one can see in Fig.2 right.

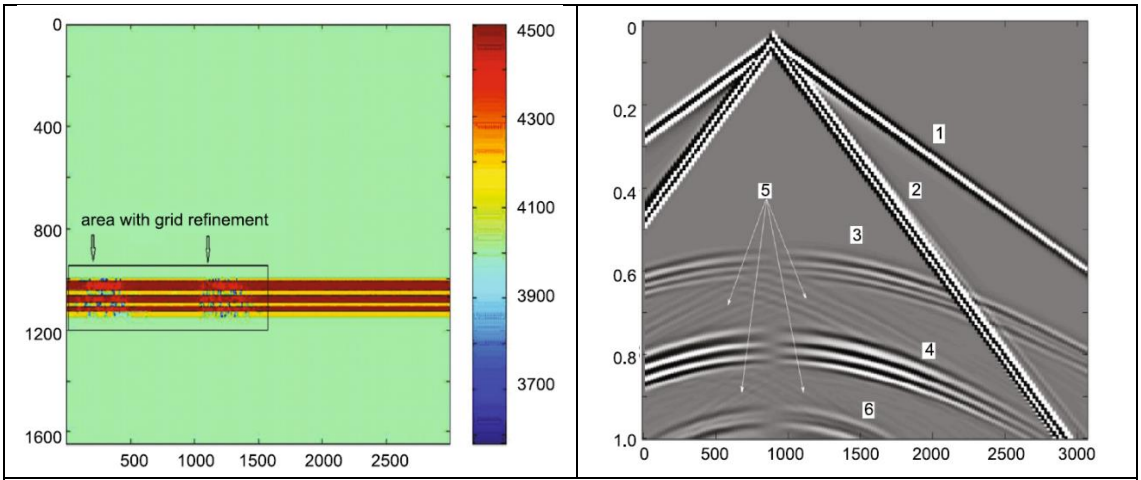


Figure 2. Left – general view of 2D model with karstic intrusions. Right – waves generating by the model. 1 – direct P-wave, 2 – direct S-wave, 3 and 4 – reflected PP- and PS-waves, 5 – scattered PP- and PS-waves, 6 – reflected SP-wave.

By comparison left and right pieces of Fig.3 one can conclude that numerical artifacts are negligible.

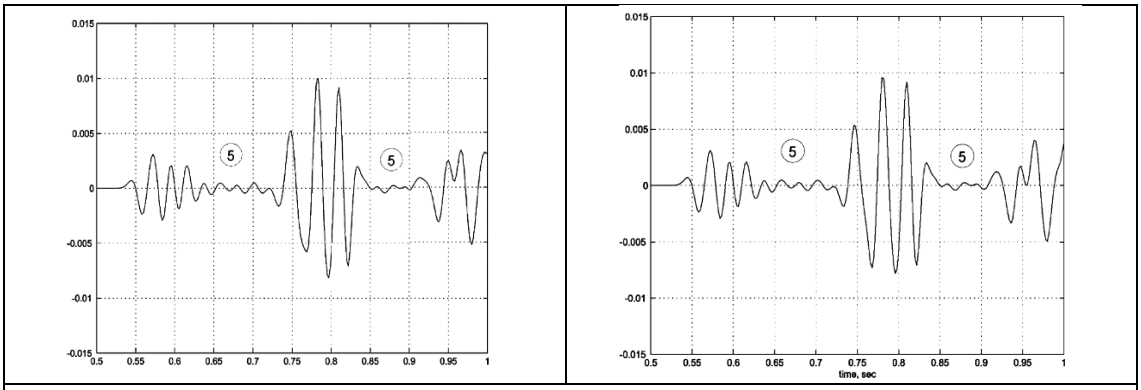


Figure 3. Central trace. Left – for uniform fine grid of 0.5 meters. Right – the same trace simulated with the coarse grid of 2.5 meters refined to 0.5 meters within target areas.

References

[1] F.Collino, T.Fouquet, P.Joly. 2003. A conservative space-time mesh refinement method for 1D wave equation. Part I: Construction. Numer. Math. V.95, 197 – 221.

FINITE ELEMENT CALCULATION OF THE EFFECTIVE THERMAL CONDUCTIVITY OF TWO-DIMENSIONAL THREE-SCALE HETEROGENEOUS MEDIA

Lucas P. Mattos[1,*], Manuel E. Cruz[2], Julián Bravo-Castillero[3]

[1]UFRJ-Federal University of Rio de Janeiro, COPPE, lucaspradomattos@gmail.com

[2]UFRJ-Federal University of Rio de Janeiro, COPPE, manuel@mecanica.coppe.ufrj.br

[3]Universidad de La Habana, jbravo@matcom.uh.cu

Heat transfer through heterogeneous materials may be modeled using sets of partial differential equations in a microscopic level where there is no heterogeneity. For this reason, the direct numerical study of such equations inside a heterogeneous medium with multiple scales can become outstandingly difficult or even impossible to perform. In the case of present interest, materials with three separate scales, one may have small particles at the smallest dimension, scattered throughout a body with the largest dimension, while forming aggregates at an intermediate dimension.

The simulation of heat conduction inside this material would require extremely fine and ill-conditioned meshes and, therefore, the success of a numerical implementation would be extremely unlikely. This is the main reason, why one proposes to calculate an effective thermal conductivity of a heterogeneous medium with multiple scales. In the present work, a numerical-analytical methodology is adopted to determine computationally the effective thermal conductivity of composite materials with two homogeneous and isotropic phases, with perfect thermal contact at the interface between them. The methodology is based on the theory of reiterated homogenization [1] and the finite element method [2].

Following the methodology description and implementation in 2-D, it is first applied to cases with known solution for validation [3]. For bilaminated composites, the computational results have matched, within round-off, the analytical effective thermal conductivity calculated in [4]. Next, results have been calculated for the two-dimensional square array of circular cylinders, which matched the semi-analytical results by Manteufel and Todreas [5] with negligible deviations.

The validated code is now applied to calculate the effective thermal conductivity of the 2-D square array of Greek crosses (figure 1). This choice is motivated by the fact, that the geometry of the Greek cross has been used in [6] as a candidate model for the microstructure of nanofluids with aggregated particles. In figure 1a, a two-scale periodic cell is depicted, while in figure 1b a three-scale cell has the same geometry in both the z and y levels. The small positive parameter ε is defined as the ratio of two successive scales, $\varepsilon = \lambda/L \ll 1$, and α is the ratio of phase conductivities, $\alpha = k_d/k_c$. The global volume fraction ϕ is defined as the total area of phase d divided by the medium total area.

The effective thermal conductivity gain for the three-scale 2-D square array of Greek crosses has been evaluated. The gain is defined as the percentage increase of the effective conductivity for the three-scale array relative to that of the two-scale array. The gain permits to identify, from the global heat transfer point of view, when it is advantageous

to dislocate material originally in the level *y* (fig 1a) and scatter it throughout the level *z* (fig 1b).

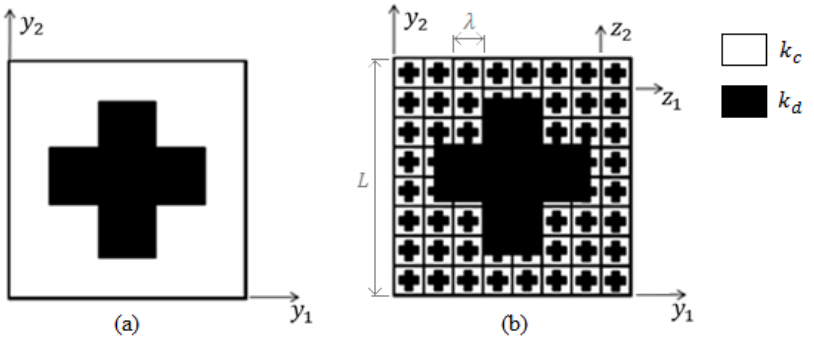


Figure 1. Periodic cell of a 2-D square array of Greek crosses with (a) 2 scales and (b) 3 scales.

The computed results are shown graphically in figure 2. The quantity ϕ_z in the horizontal axis is the local volume fraction present in the *z*-level cell. The gain has been evaluated for three different values of the global volume fraction ϕ. The results indicate, that there is an optimal local volume fraction for a maximum heat conduction gain of the three-scale array relative to the two-scale array. It is apparent, that the present numerical-analytical methodology may be a useful tool to aid interpretation of the gain in effective thermal conductivity experimentally observed with some classes of heterogeneous media.

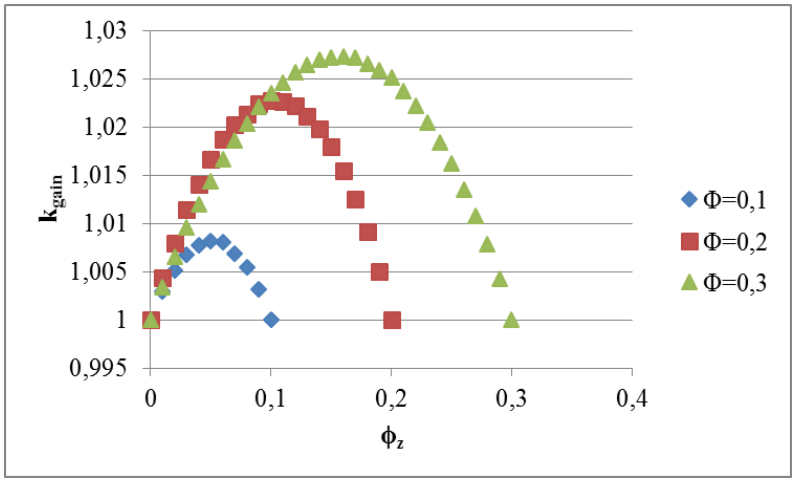


Figure 2 Effective thermal conductivity gain, k_{gain}, for the three-scale square array of Greek crosses as a function of volume fraction ϕ_z for three values of ϕ and for α=50.

References

[1] Bensoussan, A., Lions, J.L., Papanicolaou, G., 1978. Asymptotic Analysis for Periodic Structures. North-Holland, Amsterdam, The Netherlands.
[2] Hughes, T.J.R., 1987. The Finite Element Method. Prentice-Hall, Inc. New Jersey, USA.
[3] Mattos, L.P., 2017. M.Sc. Dissertation. Mechanical Eng. Program, COPPE/UFRJ.
[4] Auriault, J.L., 1983. Effective Macroscopic Description For Heat Conduction In Periodic Composites. International Journal of Heat and Mass Transfer, 26, 861–869.
[5] Manteufel, R.D., Todreas, N.E., 1994. Analytic formulae for the effective conductivity of a square or hexagonal array of parallel tubes. Int. J. Heat and Mass Transfer, 37, 647–657.
[6] Fan, J., Wang, L., 2010. Effective thermal conductivity of nanofluids: the effects of microstructure. J. Phys. D: Appl. Phys., 43, 165501 (10pp).

Multiscale Modeling of Uncertainties Associated with Material Defects and their Evolution during Deformation Processing

Rajiv Shivpuri[1,*], Sumaiya Islam[2]

[1]The Ohio State University, Columbus, Ohio, USA, Shivpuri.1@osu.edu

[2]The Ohio State University, Columbus, Ohio, USA, Islam.82@osu.edu

As the complexity and performance of engineered systems is increasing so is their susceptibility to failure risk associated with material uncertainties such as random defects. With an eye towards societal risk, engineers are required to design products and processes that offer higher performance without sacrificing safety. A major approach to risk mitigation is to either modify the defects to reduce their impact or to move them to a location with lower probability of failure.

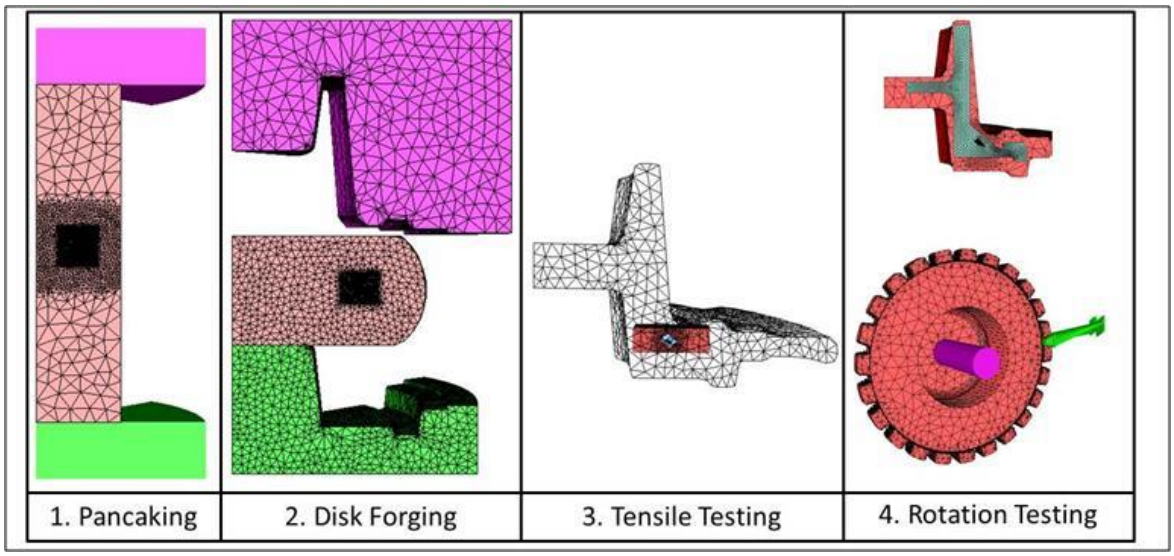
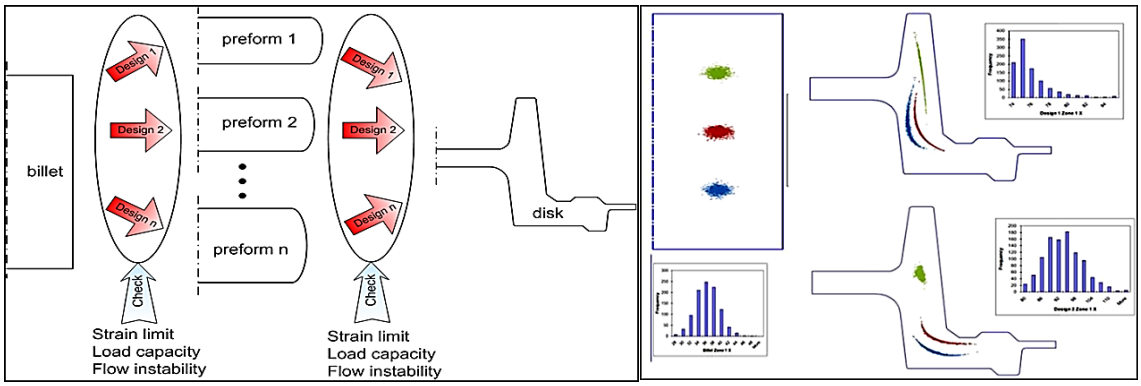


Figure 1. Embeded element RVE approach for multi-scale and multi-process analysis for linking material state to product performance

In this paper, we present a multiscale approach to model material related micro-defects, and their uncertainties during macroscale deformation processing. In this approach approach, the distribution of state variables is obtained by macro-modeling of plastic flow during multi-step deformation processing (scale ~ 10 m.) while the micro-phenomena such as stress concentrations and defect break up are modeled by embedding micro-defects (scale ~ 10 μm) in the plastic matrix. First computational challenge is to handle a scaling ratio of 10^{-6} in the FEM framework. The linking between the scales is obtained through matching the physics at the macro-level to that at the micro-level.The process design parameters (such as temperatures, velocities, preform design etc.) and the material state (defect motion and rotation during forge processing) is linked to the failure state via multibody computational modeling of the embedded inhomogeneity in a self-consistent steel matrix. As shown in Figure 1, the FEM based model uses an embedded RVE approach to characterize the evolution of defects during a individual processing as well as multi-step processing: as the billet is converted into a aeroengine disk.



(a) (b)

Figure 2. Control of plastic flow and defect distribution during deformation processing: (a) the effect of process design on plastic flow, and (b) the effect of plastic flow on location and distribution of defects..

The second computational modeling challenge comes from material defect uncertainties (location, distribution and probabilities of occurrence in the detrministic framework. To tackle this challenge, we use the deterministic framework to determine the relocation and redistribution of uncertainties due to plastic flow, and their randomness to via statistical modeling. The risk associated with defect evolution and their location is handled by "zone based" hazard models. Figure 2 (a) includes a schematic illustrating the role of process design (preforming die) in changing the deformation history of the forgign an aeroengine disk, while Figure 2(b) shows the role of this metal flwo in redistribution and relocating the defects in the forged disk.

References

[1] Pardoen, T., Scheyvaerts, F., Simar, A., Tekoglu, C., Onck, P.R., 2010. Multiscale Modeling of Ductile Failure in Metallic Alloys. C.R. Physique 11: 326-345.

[2] Coenen E.W.C., Kouznetsova V. G., Geers, M.G.D., 2012. Multi-scale continuous-discontinuous framework for computational-homogenization-localization. Journal of the Mechanics and Physics of Solids 60:1486-1507..

[3] Segurado, J., Lebensohn, R.A., Llorca, J., Tome, C.N., 2012. Multiscale modeling of Plasticity based on Embedding the Viscoplastic Self-Consistent Formulatuion in Implicit Finite Elements. International Journal of plasticity 28: 124-140.

[4] McDowell, D.L., 2008. Viscoplasticity of heterogeneous metallic materials. Material Science and Engineering R 62: 67-123.

[5] Yu, H-L., Liu, X-H., Bi, H-Y., Chen, L-Q., 2009. Deformation behavior of Inclusions in Stainless Steel Strips during Multi-pass Cold Rolling. Journal of Materials Processing Technology 209: 455 -461.

[6] Enright, M.P., McClung R.C., Huyse, L., 2005. A probabilistic Framework for Risk Prediction of Gas Turbine Engine Components with Inherent or Induced Material Anomalies. Paper GT2005-68982, Proc. of ASME Turbo Expo 2005, Reno-Tahoe, NV, USA.

[7] Claudio, R.A., Branco, C.M., Gomes, E.C., Byrne, J., Harrison, G.F., Winstone, M.R., 2004. Fatigue Life Prediction and Failure Analysis of a Gas Turbine Disc using the Finite Element Method. Fatugue Fract Engng Mater Struct 28: 849-860.

ADVANCING PREDICTIVE CAPABILITY IN BRITTLE MATERIALS THROUGH GRAPHICAL REPRESENTATIONS OF MICROSTRUCTURE

Gowri Srinivasan[1,*], Bryan Moore[2], Esteban Rougier[3], Humberto Godinez[4], Hari Viswanathan[5]

[1]Los Alamos National Laboratory, gowri@lanl.gov

[2]Los Alamos National Laboratory, bryanmoo@lanl.gov

[3]Los Alamos National Laboratory, erougier@lanl.gov

[4]Los Alamos National Laboratory, hgodinez@lanl.gov

[5]Los Alamos National Laboratory, viswana@lanl.gov

Microstructural information (fracture size, orientation, etc.) plays a key role in governing the dominant physics in fractured materials [1]. Applications of interest include dynamic fracture processes like spall and fragmentation in metals, detection of gas flow in static fractures in rock due to underground explosions, hydrofracking of methane gas from shale deposits underground etc. At relevant scales of interest, micro-fracture information can only be known in a statistical sense. The use of forward model runs that explicitly represent millions of micro-fractures to bound the uncertainty associated with these fracture statistics is computationally prohibitive, requiring thousands of runs and petabytes of information. Most approaches typically either ignore or idealize microscale information, since we lack a framework that efficiently utilizes it in its entirety to predict macroscale behavior in brittle materials.

We consider the mechanism of crack propagation in brittle materials. Unlike ductile fracture, where a large body of research exists, brittle fracture in metals is poorly understood since it occurs suddenly without warning. Recent experiments [2] have exposed the need for better predictive capability of brittle fracture and failure. This is especially relevant at high strain rates, where predicting when cracks will interact and coalesce together leading to brittle failure (spall, fragmentation) in metals remains a primary challenge. Resolving the interactions of thousands of interconnected sub-micron scale fractures (micro-cracks) while also including realistic thermo-mechanical effects like crack tip plasticity, is computationally intractable with current technologies. Each cell of a macroscale continuum simulation code could contain 10^6 micro-cracks. The entire domain can thus contain over 10^9 cracks which renders the problem computationally intractable.

In order to overcome these hurdles we have developed the next generation of fracture simulators [3] for the dynamic evolution of the fractures using graph theory. We additionally take advantage of recent advances in experimental fracture characterization that capture high-fidelity data (e.g. fracture patterns, density, aperture) to inform our models using Data Assimilation techniques. The technical challenge in both applications is similar, representing relevant physics on the graph through machine learning algorithms. Our hypothesis is that topological properties are crucial, and can be captured through a low dimensional graph representation. Predictive uncertainty is better captured through topological characteristics on the graph instead of traditional parametric methods which fail to capture subgrid effects [4].

References

[1] J. Escobedo, C. Trujillo, E. Cerreta, and E. Gray, G.T. IIIand Brown, “Effect of shock wave duration of dynamic failure of tungsten heavy alloy,” in Journal of Physics Conference Series, 2014.

[2] C. Cady, C. Adams, L. Hull, G. I. Gray, F. Prime, M.B.and Addessio, T. Wynn, and E. Papin, P.A.and Brown, “Characterization of shocked beryllium,” in EPJ Web of Conferences, 2012.

[3] H. Djijev, D. O'Malley, H. Viswanathan, J.D. Hyman, G. Srinivasan, Learning on Graphs for Predictions of Fracture Propagation, Flow and Transport, GRAML'17: First Workshop on the Intersection of Graph Algorithms and Machine Learning, Orlando, May 29- June 2, 2017.

[4] G. Srinivasan, D. Tartakovsky, B. Robinson, and A. Aceves, “Quantification of uncertainty in geochemical reactions,” Water Resour. Res.,vol. 43, 2007.H. Djijev, D. O'Malley, H. Viswanathan, J.D. Hyman, G. Srinivasan, Learning on Graphs for Predictions of Fracture Propagation, Flow and Transport, GRAML'17: First Workshop on the Intersection of Graph Algorithms and Machine Learning, Orlando, May 29- June 2, 2017.

MODELLING OF MULTI-LAYER GEOLOGIC PROFILE CONSIDERING INTRA- AND INTER-LAYER VARIABILITIES

Xuyou LI[1,*], Limin ZHANG[2]

[1]The Hong Kong University of Science and Technology. E-mail: xliar@connect.ust.hk

[2]The Hong Kong University of Science and Technology. E-mail: cezhangl@ust.hk

A geologic profile often comprises multiple material zones or has a layered structure due to complex depositional or weathering processes. Significant uncertainties are associated with the geologic profile, which can be categorized into two groups: (1) intra-layer variability, which refers to the variation of material properties within the same layer; and (2) inter-layer variability, which refers to the uncertainties associated with the interlayer boundaries. The inter- and intra-layer spatial variabilities have significant impact on the design and construction of geotechnical structures. This paper proposes an integrated random field model to characterize the inter- and intra-layer spatial variabilities of multi-layer geologic profiles simultaneously. The intra-layer spatial variability is characterized by a random field model, while the inter-layer spatial variability is characterized by a conditioned random field model. A transition zone is used to describe the gradual transition of material properties at the interlayer boundary. The proposed model is applied to characterize the spatially variable cone tip resistance at a study site, and to evaluate the effects of the integrated spatial variability of undrained shear strength on the reliability of a two-layer soil slope. Both the inter- and intra-layer spatial variabilities influence the reliability of the slope. The failure probability can be underestimated if one or both spatial variabilities are not considered. The intra-layer variability is relatively more significant for the slope example in this study. The failure probability decreases with increasing thickness of the transition zone.

UPDATING LANDSLIDE SUSCEPTIBILITY USING BAYESIAN NETWORKS

H.J. Wang[1,*], L.M. Zhang[2], X.Y. Li[3]

[1]Department of Civil and Environment Engineering, The Hong Kong University of Science and Technology, h.wang@connect.ust.hk

[2]Department of Civil and Environment Engineering, The Hong Kong University of Science and Technology, cezhangl@ust.hk

[3]Department of Civil and Environment Engineering, The Hong Kong University of Science and Technology, lixueyou@ust.hk

Landslide susceptibility assessment is essential to landslide hazard mitigation, but few attempts have been made to consider the spatial correlation among parameters in adjacent cells while conducting regional hillslope reliability analysis. This paper aims to propose a new method to update landslide susceptibility using Bayesian networks and to improve the accuracy of landslide susceptibility mapping. First, the reliability analysis model for single cells is defined. Then a Bayesian network with continuous distributed variables for an infinite slope involving failure probability and correlated influencing parameters (e.g., cohesion) is constructed. After that, the parametric correlations among cells are quantified based on random field theory and the prior probabilities for the Bayesian network. Finally, observational information is used to update the probability distributions of the parameters and the failure probability. As examples, a hypothesized infinite slope with observational information under both correlated and uncorrelated conditions is studied in this paper for illustration. Considering the failure information of certain cells decreases the stability of adjacent cells, thus the susceptibility of instability in cells is no longer independent. This method is able to consider the correlations among the computing cells and to update correlated parameters and failure probability with the integrated observational information. Hence, the landslide susceptibility becomes more reliable by taking advantage of the observational information.

SORM-BASED RBDO WITH RBFN and KRIGING

Niclas Strömberg

Örebro University, niclas.stromberg@oru.se

Recently, we have proposed a new approach for reliability based design optimization (RBDO) using second order reliability methods (SORM) [1] and a new approach for radial basis function networks (RBFN) [2]. The SORM-based RBDO formulation is solved using sequential linear or quadratic programming by performing Taylor expansions in intermediate variables defined by the iso-probabilistic transformation for mixtures of non-Gausian variables. The Taylor expansions of the reliability constraints are done at the most probable point (MPP) according to the Hasofer-Lind approach, where the MPP is found by a Newton method using an in-exact Jacobian for variables with normal, lognormal, Gumbel, gamma and Weibull distributions. The target of reliability is corrected by using four different SORM formulas: Breitung, Hohenbichler, Tvedt and a recent proposed formula. So far, the SORM-based RBDO methodology has been evaluated mostly for analytical benchmarks, showing excellent performance. For instance, a most well-known problem for two variables and 3 constraints, see Figure 1, is generalized to 50 variables with the five different distributions treated simultaneously and 75 constraints.

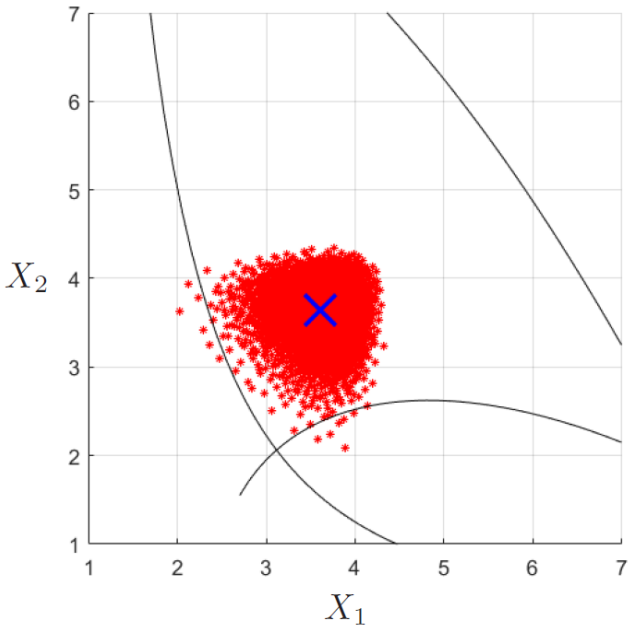


Figure 1: *This well-known benchmark for RBDO is generalized to 50 variables and 75 constraints.*

The proposed RBFN approach in [2] utilizes a bias defined a priori with a linear or quadratic regression model. In such manner, the global behavior is captured with the bias and the local behavior is tuned in by the radial basis functions. This differs from a standard approach, where the bias is defined a posterior by adding extra orthogonality constraints. In this work, we set up design of experiments (DoE) for the analytical benchmarks studied previously in [1] and then fit our RBFN to the sets of data points. Next, SORM-based RBDO with these RBFN is performed and the optimal solutions are

compared to the analytical results from [1]. This surrogate model based RBDO approach is also compared to a Kriging based RBDO approach. In this context, different strategies for DoE are also studied, e.g. latin hypercube, Halton, Hammersley, S-optimal and successive screening sampling.

References

[1] Strömberg, N., 2017. Reliability-based Design Optimization using SORM and SQP, Structural and Multidisciplinary Optimization, on-line, DOI: 10.1007/s00158-017-1679-3.

[2] Amouzgar, K. & Strömberg, N., 2016. Radial Basis Functions as Surrogate Models with a Priori Bias in Comparison with a Posteriori Bias, Structural and Multidisciplinary Optimization, on-line, DOI: 10.1007/s00158-016-1569-0.

MULTI-SCALE DESIGN METHODOLOGY FOR COMPOSITE STRUCTURES BASED ON UNCERTAINTY PROPAGATION

Ernesto Rodriguez Pila[1,*], Claire Guillebaud[1], Hervé Wargnier[1]

[1]Institut de Mécanique - Bordeax (I2M), Université de Bordeaux, UMR5295, F -33400 Talence, France

The design of a structure is clearly linked to the confidence in design choices that were made. These choices are often based on experimental and predictive analysis performed to characterize the studied structure by a complete or partial definition of properties at each scale. This study deals with the link between the product specifications and "choice leading" specifications. The aim of this work is to propose a methodology leading to the choice of designer optimising the cost of experimental and predictive developments and ensuring a high level of confidence.

Uncertainty analysis is a relevant part in the design of composite material structures. Number and scale of the structure properties to characterize and their associated level of confidence could be mastered by a better understanding of the result carried on the studied structure. Uncertainties due to manufacturing process, experimental testing and numerical modelling must be understood. Several authors treated this subject applying different statistical and computational methods to determinate variation of the response due to errors on input parameters [1-2].

At each scale of the structure, uncertainty analysis have to be performed in order to map the influence of input parameters at any scale over the result at a more complex level. Properties can be either calculated by using predictive models using properties at lower scales or doing the necessary experimental tests [3-4]. In some cases, experimental testing could be very expensive and/or complex, that is why results must give high confidence solutions. This study deals with the link between the predictive and experimental modelling pyramid (Figure 1) and the product specifications.

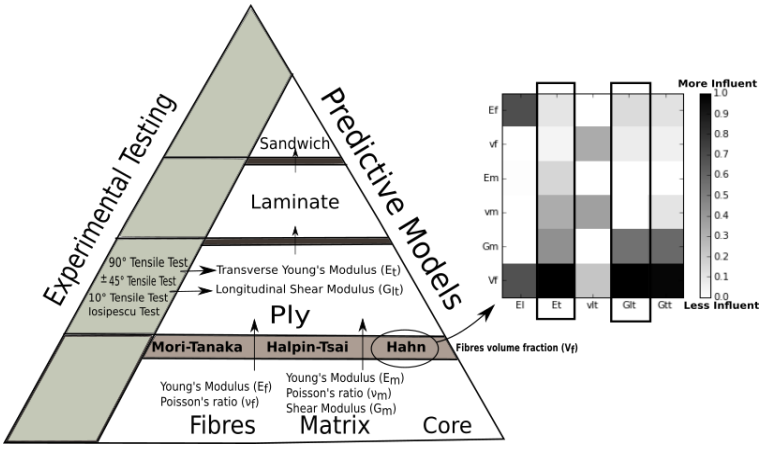


Figure 1 Modelling pyramid

In the case of composite materials, guiding designer during modelling process is important. Indeed, the designer has to perform multi-scale analysis in order to characterize the structure. The designer must chose between testing or simulations to define all significant properties of the structure. These choices and the requested level of

confidence define modelling paths that could be followed in order to optimize the trade-off between modelling cost and uncertainty.

Using a genetic algorithm allows to evaluate a great number of different modelling paths and to find a low modelling cost and low uncertainty solution. The designer is able to modify the objective fonction if he considers relevant getting a solution with lower uncertainty increasing slightly the cost or vice versa. The genotype is defined by all necessary parameters used to characterize the structure at all scales. Each gene in the genotype can take different values which indicate if the property is evaluated by an analytical model, an experimental model or if it is taken from a database.

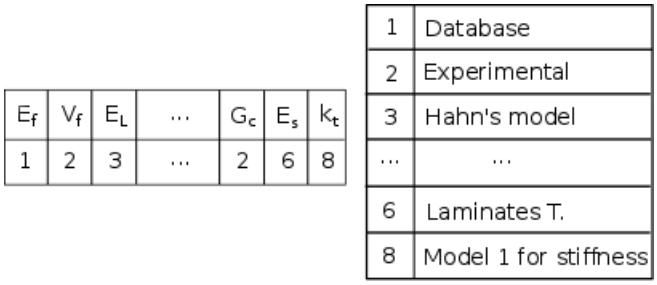


Figure 2 Example of the proposed genotype for a sandwich bending beam

The methodology was implemented to the case of a sandwich bending beam (Figure 2). Using a defined geometry and proposing structure specifications, methodology is capable to propose several modelling paths as solutions. Each solution is analysed to find an optimal with a balance between cost and response uncertainty. The methodology is about to be applied to a complex structure and numerical models will be added.

References

[1] C. Conceição António and L. N. Hoffbauer, “Uncertainty analysis on sensitivity applied to angle-ply composite structures,” Reliability Engineering & System Safety, vol. 92, pp. 1353-1362, 2007.

[2] A. K. Noor, J. H. Starnes et J. M. Peters, “Uncertainty analysis of composite structures, ” Computer Methods in Applied Mechanics and Engineering, vol. 185, 2000

[3] Kim, Hyonny, D. Whisler, Z. M. Chen, C. Bisagni, M. Kawai, et R. Krueger. Proceedings of the American Society for Composites 2014-Twenty-Ninth Technical Conference on Composite Materials. DEStech Publications, Inc, 2014.

[4] Breuer, Ulf Paul. Commercial Aircraft Composite Technology. Springer, 2016.

PREDICTIVE MODELING FOR BRITTLE METAL FRACTURE GROWTH

Bryan Moore[1*], Esteban Rougier[2], Gowri Srinivasan[3], Daniel O'Malley[4]

[1]Los Alamos National Laboratory, bryanmoo@usc.edu

[2]Los Alamos National Laboratory, erougier@lanl.gov

[3]Los Alamos National Laboratory, gowri@lanl.gov

[4]Los Alamos National Laboratory, omalled@lanl.gov

Currently, there are multiple models [1] that can accurately simulate microstructure or macrostructure fracture propagation in brittle materials. In the microscale region, fracture properties (fracture geometry, coalescence, etc.) are vital in understanding the structural stability of a material. Incorporating microstructural knowledge within a macroscale fracture model is computationally infeasible, necessitating petabytes of data and large-scale computing resources. Thus, a major problem beyond effectively modeling fracture propagation at multiple scales is bridging the gap between these models in an efficient matter.

Furthermore, varying strain rates on brittle materials can vastly change the behavior of fracture growth and the time to complete material failure. Much of the past work in coupling these multi-scale models applied the separation of scales principles [2]. This assumption, however, fails in zones of high strain and damage. Many brittle materials are subjected to high strain rates (Carbon fiber/titanium on jets, space shuttles, etc.) over an extended period and material failure would be catastrophic. Building a model, or ensemble of models, that can accurately predict material properties under a wide range of strain rates is crucial to the understanding and construction of future brittle metals.

In our approach, we have implemented a Machine Learning (ML) and graph theory framework to generate the link between the micro and macro-scale models. Fracture information is represented by a graphical model to reduce the dimensionality of the fracture formation and discover how fracture networks develop [3]. ML algorithms are subsequently trained on the graphical representations, with the ground truth being the high-fidelity model calculations. A finite element software, the Hybrid Optimization Software Suite (HOSS), is deployed as the ground truth model due to its highly accurate results for fracture physics within the high strain rate regime [4]. Multiple ML models will be developed to cover the large range of strain rates that a brittle material may be subject to. This framework will couple the recent successes in ML and graph theory while preserving the physical intuition present in the existing dynamic fracture models.

References

[1] Lawn, B., Fracture in Brittle Solids 2nd Edition Cambridge: Cambridge University Press, 1993

[2] Coenen, E.W.C., Kouznetsova, V.G., Bosco, E. et al. Int J Fract (2012) 178: 157. doi:10.1007/s10704-012-9765-4

[3] Jordan, Michael Irwin, ed. *Learning in graphical models*. Vol. 89. Springer Science & Business Media, 1998.

[4] Rougier E, Knight EE, Broome S, Sussman A, Munjiza A. Validation of a three-dimensional Finite-Discrete Element Method using experimental results of the Split Hopkin-son Pressure Bar test. Int. J. Rock Mech. Mining Sci. (2014); 70: 101–108.

EFFECT OF LOCAL FIBER VOLUME FRACTION VARIABILITY AND MISALIGNMENT OF FIBERS ON STIFFNESS AND FAILURE OF UD CARBON FIBER COMPOSITE PLY

Fabio Malgioglio[1,*], Anna Matveeva[2], Francisco Mesquita[3], Christian Breite[4], Yentl Swolfs[5], Laszlo Farkas[6], Wim Desmet[7], Stepan V. Lomov[8]

[1]Siemens Industry Software NV, fabio.malgioglio@siemens.com

[2]Siemens Industry Software NV, anna.matveeva@siemens.com

[3]Department of Materials Engineering, KU Leuven, francisco.mesquita@kuleuven.be

[4]Department of Materials Engineering, KU Leuven, christian.breite@kuleuven.be

[5]Department of Materials Engineering, KU Leuven, yentl.swolfs@kuleuven.be

[6]Siemens Industry Software NV, laszlo.farkas1@siemens.com

[7]Department of Mechanical Engineering, KU Leuven, wim.desmet@kuleuven.be

[8]Department of Materials Engineering, KU Leuven, stepan.lomov@kuleuven.be

Thanks to their advanced mechanical properties and low density, composite materials are commonly employed in aerospace and automotive components. Due to the intrinsic complexity of such materials, i.e. the presence of different phases, their behavior and damage prediction is quite complex. Today, to support the design process, computer simulations are commonly used together with expensive experimental campaigns, which are necessary for the material characterization. Usually experiments present a certain variability in the results, which is partially due to the intrinsic material variability occurring at different scales. Each single fiber, for example, has different properties, e.g. strength, which can be described by a probability distribution. The fiber volume fraction, generally considered uniform for unidirectional (UD) materials, shows variations at the microscale because fibers tend to pack together with a random arrangement. This results in areas where the fiber density is higher or lower with respect to the average value. The volume fraction variation due to the random packing of fibers is of particular interest because it influences the local material stiffness and local stress distribution, which drive the composite failure. Furthermore, fibers present a small angle variation with respect to the nominal direction, which affect the local stiffness.

In this paper, a non-deterministic and multi-scale virtual testing approach for the prediction of stiffness and strength of UD composites is presented. In the proposed method, the variabilities of fiber strength, fiber volume fraction and fiber misalignment are considered at different scales of interest. Several FE models of virtual specimens of UD carbon fiber/epoxy prepreg plies are generated and meshed with 3D solid elements. For every realization, the local fiber volume fraction and misalignment are randomly assigned to each mesh element, accounting for spatial correlation, which were studied in [1,2]. Local homogenized elastic properties of each mesh element are derived analytically using Chamis formulae [3] based on the local volume fraction in local coordinate systems (CS), which depend on the fiber misalignment. The strenght of each element is assumed to be equal to the strength of a fiber bundle with the same volume fraction. Hence, the strength probability distributions of fiber bundles with different volume fractions are

precomputed with a micromechanical model proposed by Swolfs et al [4,5]. The model considers bundles of randomly distributed fibers [6,7] and is able to describe the propagation of fiber breaks up to the final bundle failure. The generated virtual specimes are tested in tension in the fiber direction. As a result, Young's modulus of the material and tensile strength are determined at the ply level together with their scatter. Predicted composite Young's modulus and strength distributions are compared with existing experimental data from literature [8].

In the current formulation, failure modes other than fiber tensile failure are not considered. However, this paper is part of a broader research activity aimed to establish a non-deterministic industrial multi-scale methodology for the full behavior and damage prediction of UD composite materials. One of the outcomes of this work, is to extend the capabilities of the VMC ToolKit integrated in the Siemens PLM Software [9] towards stochastic effects and computing composite strength.

The authors acknowledge the FiBreMod ITN project, European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 722626, SIM (Strategic Initiative Materials in Flanders) and VLAIO (Flemish government agency for Innovation and Enterpreneurship) for their support of the ICON M3Strength project, which are part of the research program MacroModelMat (M3).

References

[1] SHR Sanei, RS Fertig III. Uncorrelated volume element for stochastic modeling of microstructures based on local fiber volume fraction variation, Compos.Sci.Technol. 117 (2015) 191-198.
[2] MPF Sutcliffe, SL Lemanski, AE Scott. Measurement of fibre waviness in industrial composite components, Composites Sci.Technol. 72 (2012) 2016-2023.
[3] CC Chamis. Mechanics of composite materials: past, present, and future, Journal of Composites, Technology and Research. 11 (1989) 3-14.
[4] Y Swolfs, Hybridisation Of Selfreinforced Composites: Modelling And Verifying A Novel Hybrid Concept, PhD Thesis (2015).
[5] Y Swolfs, I Verpoest, L Gorbatikh, Issues in strength models for unidirectional fibre-reinforced composites related to Weibull distributions, fibre packings and boundary effects, Composites Science and Technology. 114 (2015) 42-49.
[6] A Melro, P Camanho, S Pinho. Generation of random distribution of fibres in long-fibre reinforced composites, Composites Sci.Technol. 68 (2008) 2092-2102.
[7] V Romanov, SV Lomov, Y Swolfs, S Orlova, L Gorbatikh, I Verpoest. Statistical analysis of real and simulated fibre arrangements in unidirectional composites, Compos.Sci.Technol. 87 (2013) 126-134.
[8] R Degenhardt, A Kling, A Bethge, J Orf, L Kärger, R Zimmermann, et al. Investigations on imperfection sensitivity and deduction of improved knock-down factors for unstiffened CFRP cylindrical shells, Composite Structures. 92 (2010) 1939-1946.
[9] L Farkas, K Vanclooster, H Erdelyi, R Sevenois, SV Lomov, T Naito, et al., Virtual material characterization process for composite materials: an industrial solution, 17th European Conference on Composite Materials (ECCM17) (2016).

Fluctuating Hydrodynamics of Complex Fluid Mixtures

Aleksandar Donev[1,*], Andy Nonaka[2], John Bell[2], Alejandro Garcia[3,2]

[1]Courant Institute, New York University, New York, NY, donev@courant.nyu.edu

[2]Lawrence Berkeley National Labs, Berkeley, CA, AJNonaka@lbl.gov, JBBell@lbl.gov

[3]San Jose State University, San Jose, CA, algarcia@algarcia.org

Thermal fluctuations in fluid dynamics arise from the fact that fluids are composed of molecules whose positions and velocities are random. Because they span the whole range of scales from the microscopic to the macroscopic, fluctuations need to be consistently included in all levels of description. Fluctuating hydrodynamics is a powerful tool for modeling of nonequilibrium phenomena at the mesoscale, where it is no longer possible to use fully atomistic models, but where fluctuations still need to be explicitly modeled. The continuum equations of fluctuating hydrodynamics (FHD) are a very challenging multiscale, or more precisely, many-scale system of stochastic partial differential equations. Fast sound wave modes (pressure fluctuations) make the compressible equations stiff and require the introduction of low Mach number fluctuating models [1,4]. There is often a very large separation of time scales between different physical processes, for example, mass diffusion in realistic fluids is much slower than momentum or heat diffusion. Similarly, there is often a large separation of length scales as well, for example, the Debye length in electrolyte solutions [4] is much smaller than relevant problem scales.

This talk will contain a review of our recent work on computational FHD of complex multispecies liquid mixtures.

In [1] we developed a low Mach number FHD formulation describing transport of mass and momentum in a multispecies mixture of incompressible miscible liquids at specified temperature and pressure. The formulation applies to non-ideal mixtures of arbitrary number of species, without the need to single out a 'solvent' species. We studied the development of giant nonequilibrium concentration fluctuations in a ternary mixture subjected to a steady concentration gradient. We numerically studied the development of diffusion-driven gravitational instabilities (triggered by thermal fluctuations) in a ternary mixture, and favorably compared our numerical results to recent experimental measurements in a Hele-Shaw cell.

Presenting Author, Second Author, Third Author

In [2] we formulated and studied computationally the compressible FHD equations for reactive multi-species fluid mixtures. We studied the suppression of non-equilibrium long-ranged correlations of concentration fluctuations by chemical reactions, as well as the enhancement of pattern formation by spontaneous fluctuations. In [3] we developed numerical methods for FHD of reaction-diffusion systems. The FHD description naturally extends from the regime where fluctuations are strong, i.e., each hydrodynamic cell has few (reactive) molecules, to regimes with moderate or weak fluctuations, and ultimately to the deterministic limit. We demonstrated and quantified the importance of thermodynamic fluctuations to the formation of a two-dimensional Turing-like pattern, and examined the effect of fluctuations on three-dimensional chemical front propagation, to show that fluctuations accelerate pattern formation in spatially homogeneous systems, and lead to a qualitatively-different disordered pattern behind a traveling wave. In ongoing work that will be discussed, we propose a low Mach FHD formulation for reactive mixtures that combines the methods developed in [1] and [3]. We study the development of a gravitational instability at the front of an acid-base reaction, and compare to recent experiments in the group of Anne De Wit.

In recent work [5], we have formulated and studied computationally the low Mach number fluctuating hydrodynamic equations for (non-reactive) electrolyte solutions. This enables the study of hydrodynamic transport in mixtures of charged species at the mesoscale, down to scales below the Debye length, where thermal fluctuations have a significant impact on the dynamics. In the stochastic setting, our model captures the predicted dynamics of equilibrium and nonequilibrium fluctuations. We also identify and model an instability that appears when diffusive mixing occurs in the presence of an applied electric field. Future work will include chemical reactions, as required to model charge effects in acid-base reactions, as well as weak electrolytes.

References

[1] A. Donev and A. J. Nonaka and A. K. Bhattacharjee and A. L. Garcia and J. B. Bell. Low Mach Number Fluctuating Hydrodynamics of Multispecies Liquid Mixtures, Physics of Fluids, 27(3):037103, 2015.

[2] A. K. Bhattacharjee, K. Balakrishnan, A. L. Garcia, J. B. Bell and A. Donev. Fluctuating hydrodynamics of multispecies reactive mixtures, J. Chem. Phys., 142, 224107, 2015.

[3] C. Kim, A. Nonaka, J. B. Bell, A. Garcia and A. Donev. Stochastic Simulation of Reaction-Diffusion Systems: A Fluctuating-Hydrodynamics Approach, J. Chem. Phys., 146, 124110, 2017.

[4] J.-P. Peraud, A. Nonaka, A. Chaudhri, J. B. Bell, A. Donev and A. L. Garcia, Low Mach Number Fluctuating Hydrodynamics for Electrolytes, Phys. Rev. F, 1(7):074103, 2016.

CHRACTERIZING TEMPORAL AND SPATIAL VARIABILITY IN SOIL-VEGETATION-ATMOSPHERE-TRANSFER (SVAT) MODELLING OF RECLAMATION COVERS IN NORTHERN ALBERTA, CANADA

Md. Shahabul Alam[1,*], Mingbin Huang[2], Sidney Lee Barbour[3], Bingcheng Si[4]

[1]Department of CGE, University of Saskatchewan , Canada, msa181@mail.usask.ca

[2]Department of CGE, University of Saskatchewan, Saskatoon, hmingbin@yahoo.com

[3]Department of CGE, University of Saskatchewan, Saskatoon, lee.barbour@usask.ca

[4]Department of Soil Science, University of Saskatchewan, Saskatoon, bing.si@usask.ca

A long-term (60 y) water balance of reclamation covers at Syncrude Canada's Aurora oil sands mine in northern Alberta, Canada has been simulated using soil-vegetation-atmosphere-transfer (SVAT) numerical models. Historically, SVAT models are calibrated and validated against short-term (<10y) monitoring data from a single location. The calibrated models are used to evaluate the long-term performance of potential cover designs using long-term (60 y) historical climate data. Given that these covers are constructed over 10s-100s of ha it is to be expected that variability in material handling and construction methods will create variabilitiy in soil properties (e.g., saturated hydraulic conductivity, K_s). The soil properties are also known to evolve over time as a result of vegetation growth, settlement, and weathering processes (e.g. freeze/thaw and wet/dry cycling).

The study site at Syncrude's Aurora Capping Study (ACS) includes 12 cover designs replicated three times (36 one-hectare cells) and constructed over lean oil sands (LOS) overburden. A single profile of instrumentation within each cell has been used to monitor soil water, soil temperature, and soil suction since 2013. This study focuses on 4 of the cover designs which contain the same 3 soil types (salvaged peat and sandy subsoil overlying LOS mining waste). SVAT models (i.e., HYDRUS-1D) were calibrated indepedendently for each of the replicate cells and for each of 4 alternative cover designs (total of 12 calibration data sets), and also undertaken independently for the consecutive years of monitoring (2013-2016).

Five soil parameters (Θ_r, Θ_s, α, n, and K_s) for each soil type (Peat, subsoil, and LOS) were optimized using the inverse modelling against the measured soil water contents. The differences in the optimized parameter values for the same soil type at the same cell across the 4 years were atrributed to temporal uncertainty while the differences in the optimized parameters for the same soil type at various locations (i.e., cells) were used to represent spatial uncertainty. The optimized values of K_s obtained from the calibration were compared with those measured directly at the sites using Guelph permeameter (GP, K_{fs} measurements) and air peameater (AP, K measurements).

The standard deviation (STD) and coefficient of variance (CV) of all cells and years, representing overall parameter variability, is shown in Table 1. The parameter with the highest overall uncertainty was K_s, which is indeed known to be a highly variable material property. The STD and CV values of each optimzed parameter calculated based on the mean of each optimized parameter at each cell were used to represent the spatial uncertainty of each model parameter (Table 2). It is clear from Table 2 that the spatial variability had the largest contribution to the overall parameter uncertainty for K_s.

Table 1. The STD and CV of each optimized parameter using all optimized values at all cells

Soil	Θ_r (cm^3/cm^3)		Θ_s (cm^3/cm^3)		α (1/cm)		n		Log (Ks) (cm/d)	
	STD	CV	STD	CV	STD	CV	STD	CV	STD	CV
Peat	0.027	57.6	0.053	8.9	0.018	36.2	0.105	9.0	0.34	-7.2
Subsoil	0.019	124.6	0.038	10.4	0.007	24.4	0.202	9.7	0.35	-7.5
LOS	0.036	55.1	0.052	13.4	0.009	20.6	0.206	11.3	0.76	-11.2

Table 2. The STD and CV of each optimized parameter calculated using the mean at each cell for the same material.

Soil	Θ_r (cm^3/cm^3)		Θ_s (cm^3/cm^3)		α (1/cm)		n		Log (Ks) (cm/d)	
	STD	CV	STD	CV	STD	CV	STD	CV	STD	CV
Peat	0.019	41.1	0.050	8.5	0.015	30.3	0.085	7.3	0.28	-6.0
Subsoil	0.015	98.2	0.036	9.7	0.007	23.6	0.194	9.2	0.34	-7.3
LOS	0.031	47.0	0.042	11.0	0.007	17.6	0.188	10.3	0.58	-8.8

The variability in K_s as defined by the model optimization can be compared to that defined using direct field measurements of K_s using GP or AP. As shown in Figure 1 below, the optimized K_s values for peat and subsoil were generally lower than those obtained from GP measurements; however, they fall in the same order of magnitude (Figure 1). The optimized K_s values for subsoil and LOS were also lower than those measured by the AP as explained by Huang et al. (2016), while the optimized K_s values for peat were found very similar to the AP measurements. The optimized K_s values for LOS were also similar to the GP measured values. Most importantly, the optimized and measured K_s distributions are similar indicating that the optimization methods are capturing the same degree of spatial variability in K_s as that obtained from the direct measurements of K_s.

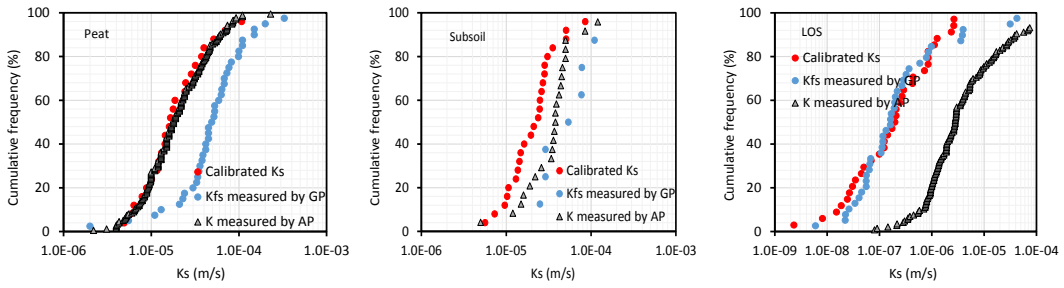


Figure 1. The distributions of optimized K_s, measured field saturated K_{fs} using GP and K using AP for peat, subsoil, and LOS by OKC (OKC, 2013).

Interstingly, a comparision of the optimized and measured values of K_s obtained for the same test cell did not have a strong correlation ($R^2 < 0.01$). This suggests that the variation in the K_s values for LOS was occuring over spatial scales smaller than the size of a cell.

References

[1] Huang et al., 2016. Characterizing the spatial variability of the hydraulic conductivity of reclamation soils using air permeability. Geoderma 262:285-293.

[2] O'Kane Consultants Inc., 2013. Aurora soil capping study of cover system materials characterization program-hydraulic conductivity testing. OKC report No. 690/99-03.

BLACK BOX OPTIMIZATION OF 3D INTEGRATED SYSTEMS

Hakki M. Torun[1], Madhavan Swaminathan[2,*]

[1,2]School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta,GA

[1]htorun3@gatech.edu, [2]madhavan.swaminathan@ece.gatech.edu

System Details:

3D integration has become a popular technique among the system integration community to overcome electrical performance and density problems. As the transistor density increases, however, it raises new challenges in design of 3D integrated circuits (3D ICs) such as modeling, fabrication and thermal management. In order to simulate the electrical and thermal performance of the system, a solver using finite volume method has been developed to to solve for the voltage and temperature distributions [1]. This electrical-thermal solver uses 3D nonuniform mesh and domain decomposition to capture the multi-scale geometries. This is then combined with a circuit solver to estimate temperature dependent clock skew. In [2], authors have demonstrated use of Machine Learning, namely Bayesian Optimization(BO) for 3D ICs, consisting of stacked dies, interposer and printed circuit boards for optimkization. In this paper, we propose a 2-stage BO algorithm that acquires necessary parameters to minimize temperature gradient of a 3D IC by relying on electrical-thermal solver for simulations. The problem is posed as a 5 dimenionsal problem which includes heat transfer coeeficient, Thermal Interface Material (TIM), TIM thickness, Underfill material and printed circuit board material.

Bayesian Optimization for Black Box Optimization:

In majority of black-box systems, including 3D ICs, it is not possible directly to access gradient information at a point. In BO based on Gaussian Processes (GP), gradient information is not required, hence, it is a suitable and promising candidate for black box optimization. In BO, the function to be optimized is represented as a joint, multi-dimensional GP with a mean (μ) function and convariance (K) matrix, given by:

$$f(\boldsymbol{x}) = \mathcal{N}\big(\mu(\boldsymbol{x}), K(\boldsymbol{x})\big) \quad (1)$$

where x represents the *D* dimensional input vector and for *M* observations can be written as $x = (x_1, x_2, \dots, x_M)$. As it is assumed there is no prior information about the underlying function, we use one of the popular kernel functions used in literature, *automatic relevance determination (ARD) Matern 5/2 function*, given as:

$$K(\boldsymbol{x}) = \begin{bmatrix} k(x_1,x_1) & \cdots & k(x_1,x_M) \\ \vdots & \ddots & \vdots \\ k(x_M,x_1) & \cdots & k(x_M,x_M) \end{bmatrix} \quad k(x_i,x_j) = \sigma_f^2\left(1+\sqrt{5}\,r+\frac{5}{3}r^2\right)e^{(-\sqrt{5}r)} \quad (2)$$

where $r = \left(\sum_{d=1}^{D} \frac{(x_{i,d}-x_{j,d})^2}{\sigma_d^2}\right)^{1/2}$; σ_f and σ_d are hyperparameters of $K(\boldsymbol{x})$.

The traditional approach of BO is obtaining an acqusition function (*u(x)*) based on pre-defined strategy and use auxillary optimization on this acquisition function to find the new query point, x_{M+1}. Note that optimizing *u(x)* doesn't require additional queries, but use the knowledge of previous samples to get a prediction at candidate points using:

$$\mu(x_{M+1}) = k^T K^{-1} f_{1:M} \qquad \sigma^2(x_{M+1}) = k(x_{M+1}, x_{M+1}) - k^T K^{-1} k \quad (3)$$

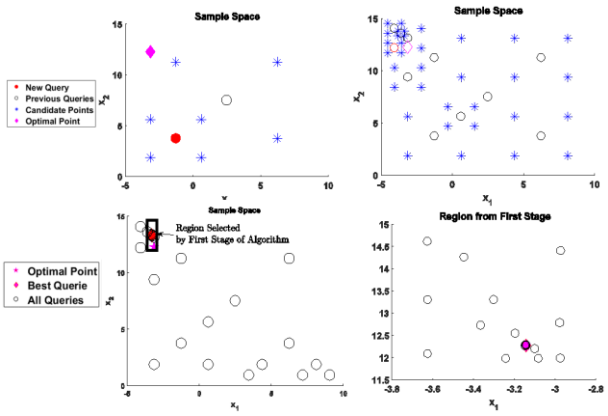


Figure 1: Flow of Algorithm for Branin function

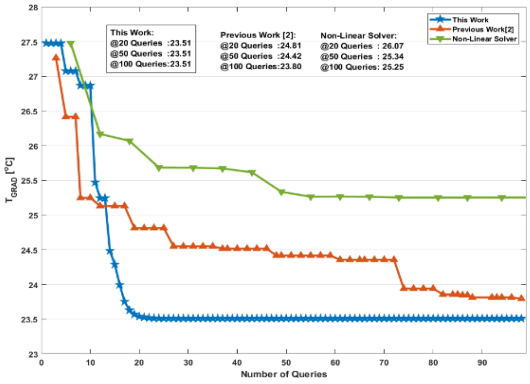


Figure 2: Performance Comparison

In [2], a BO algorithm with exponential convergence (IMGPO) [3], is used to optimize performance of 3D ICs and its superiority over other methods such as non-uniform optimization and pattern search, is shown.

2-Stage Bayesian Optimization Algorithm:

The new algorithm we present consists of 2-stages: exploration/exploitation and pure exploitation. In the first stage, the sample space is divided into 2 *D* regions and candidate points, chosen at center of each region, are generated. Then, u(x) is evaluated at candidate points and a new region is selected, wich then gets divided furhter into 2 *D* regions and added to total regions. At each iteration, one of the three popular acquisition functions, PI, EI and UCB, are used sequentially, similar to [4]. Then, the acqusition function providing 'largest gain' is chosen and algorithm continues using this function. The first stage remains until it explores a small enough region such that the euclidian distance between 'previous maxima' and 'current maxima' are negligible. Then, the second stage starts with this 'small region' and 'best acquistion function' provided by the first stage and finds the global maxima (or minima), with dividing provided along 3 new regions along its longest coordinate. The progression of the algorithm for 2-D Branin-Hoo function is shown in Figure 1.

Each function query, corresponding to simulation of a multi-scale, high-dimensional system, requires substantial CPU time. The proposed algorithm is shown to be promising for reducing total design time of such systems by converging to the minima with minimum function queries, where a decrease of 50 samples compared to IMGPO for the 3D IC case is possible, as shown in Figure 2.

References

[1] Xie, J., Swaminathan, M. (2011). Electrical-thermal co-simulation of 3D integrated systems with micro-fluidic cooling and Joule heating effects. *IEEE Transactions on Components, Packaging and Manufacturing Technology*, *1*(2), 234-246.

[2] Park, S. J., Bae, B., Kim, J., & Swaminathan, M. (2017). Application of Machine Learning for Optimization of 3-D Integrated Circuits and Systems. *IEEE Transactions on Very Large Scale Integration (VLSI) Systems*.

[3] Kawaguchi, K., Kaelbling, L. P., & Lozano-Pérez, T. (2015). Bayesian optimization with exponential convergence. In *Advances in Neural Information Processing Systems*

[4] Hoffman, M. D., Brochu, E., & de Freitas, N. (2011, July). Portfolio Allocation for Bayesian Optimization. In *UAI* (pp. 327-336).

PLASTICITY AND FRACTURE IN QUASI-BRITTLE METALS

Abigail Hunter[1,*], Len Margolin[2]

[1]Los Alamos National Laboratory, ahunter@lanl.gov

[2]Los Alamos National Laboratory, len@lanl.gov

Many have considered the propagation of penny-shaped cracks in brittle materials. In this case, crack growth is typically attributed to the breaking of atomic bonds at the crack tip. In the case of metals, and in particular quasi-brittle metals, plasticity also occurs near the crack tip in a region called the process zone. This plastic region is often neglected since modeling atomic bond breakage, dislocation motion, and crack growth quickly becomes a very complicated multiscale problem, particularly on the continuum scale where micro- and meso-scale mechanisms cannot be explicitly accounted for.

Additionally, high strain rate (10^3 s^{-1} and above) loading can drastically change the overall material response. Constitutive models that can accurately account for material strength and damage evolution under high rate loading conditions are essential for simulations of explosively-driven systems, hypervelocity impacts, and more generally, material deformation and failure under shock wave loading.

In this work, we focus on development of a constitutive model for fracture in brittle and quasi-brittle metals. In particular, we consider crack growth in these metals under a range of loading rates. We build off of Griffith's energy criterion [1], which states that crack growth will occur in the case that the strain energy released by growth exceeds the surface energy required to form new crack surface during growth. Similar to the previous work of Barenblatt [2], Dugdale [3], Rice [4], Olesiak and Wnuk [5], and others, we consider a plastic process zone at the crack tip that impacts how the crack will grow. We investigate the varied effect this localized plastic region will have on crack growth as the loading rate changes. This may be responsible for such phenomena as the ductile-brittle transition seen in the stress-strain curves of quasi-brittle metals.

References

[1] Griffith, A.A., 1921. The Phenomena of Rupture and Flow in Solids. Philosophical Transactions of the Royal Society A 221, 582-593.

[2] Barenblatt, G.I., 1962. The Mathematical Theory of Equilibrium Cracks Formed in Brittle Fracture. Advances in Applied Mechanics 7, 55-129.

[3] Dugdale, D.S., 1960. Yielding of Steel Sheets Containing Slits. Journal of the Mechanics and Physics of Solids 8, 100-104.

[4] Rice, J.R., 1968. A Path Independent Integral and the Approximate Analysis of Strain Concentration by Notches and Cracks. Journal of Applied Mechanics 35, 379-386.

[5] Olesiak, Z., Wnuk, M., 1968. Plastic Energy Dissipation due to a Penny-Shaped Crack. The International Journal of Fracture Mechanics 4, 383-396.

HIGH-ENTROPY ALLOYS: MAXENT MODELLING AND ELASTICITY CALCULATION

S. Q. Wang

Shenyang National Laboratory for Materials Science, Institute of Metal Research, CAS, Shenyang 110016, P. R. China

The importance of entropy in the structure formation of condensed matters is convincingly exemplified by the recent discovery of high-entropy alloys (HEAs) [1]. The determination of these alloys' atomic structures of is considered as the typical multi-uncertainty problem due to the extremely random occupations of different elements on the lattice sites. The high configurational entropy acts as the decisive role in HEA phase solidification. The atomic structure model is commonly created through finding the optimized configuration with the minimum system energy for the traditional alloys in theoretical studies. However, the maximum entropy configuration in line with the principle of maximum entropy (MaxEnt) should be the first consideration in HEAs modelling. The HEAs bulk models had been successfully created through MaxEnt principle, and the paracrystalline lattice property of these alloys was studied by molecular mechanics simulations [2,3]. In this work, the supercell models with periodic boundary condition are created for several quinary and senary HEAs by MaxEnt modelling. With the built models, the elastic constants of these HEA alloys are calculated by first-principles calculation within the framework of the density-functional theory.

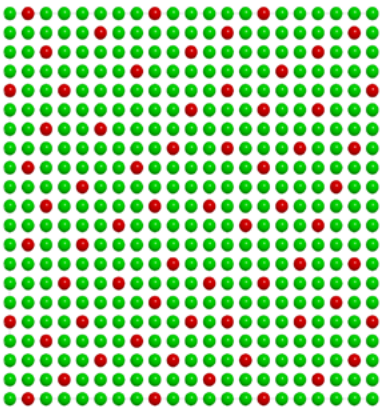


Figure 1: Periodic MaxEnt model of 2D A_xB_{1-x} (x=0.15) random-substitution alloy.

The procedure of the MaxEnt model building in this study is similar to our previous work [3], except that a periodic boundary condition is used to convenience for DFT calculation. Figure 1 shows the periodic MaxEnt model of 2D A_xB_{1-x} (x=0.15) random-substitution alloy in a 20×20 square lattice for an illustration of the technique. A series of n×n×n MaxEnt models with n=2, 3, 4 and 5 are created for FCC CoCrFeMnNi and BCC AlCoCrFeNi HEAs. The elastic constants of these models are calculated by using the cell-volume-unrestricted energy-strain method [4]. The elastic constants of the HEA phases are obtained from these theoretical results through numerical data interpolation. The synergistic effect in the elements movement is observed during the structure deformation under strain in these HEA phases.

This work was supported by the National Natural Science Foundation of China (No.51471164) and the National Key R&D Program of China (No.2016YFB0701302).

The abstract should be written in English and it should be maximum two pages. All the abstarct should be single spaced. Font types and sizes should follow this template. Table 1 provides some information for preparation of the abstarct.

Table 1. Details of the abstract prepartion

Abstract number of pages	Title font	Authors font	Affiliations font	Table and Figure captions	Table contents	References
Maximum 2	Times New Roman – 12 pt – capital – bold	Times New Roman – 11 pt – bold	Times New Roman – 10 pt	Times New Roman – 11 pt	Times New Roman – 10 pt	Times New Roman – 11 pt

Table captions should be given above tables and Figure captions should be given below the Figures. Both captions should be centered.

References

[1] J. W. Yeh, *et. al.*, Adv. Eng. Mater. **6**, 299 (2004).
[2] S. Q. Wang, AIP Advances. **3**, 102105 (2013).
[3] S. Q. Wang, Entropy. **15**, 5536 (2013).
[4] S. Q. Wang, H. Q. Ye, Phys. Stat. Sol. **240**, 45 (2003).

Calculation of Small failure probability in slopes with spatial variation of soil properties

Xianfeng Luo[1], Xin Li[2,*], Tao Cheng[1]

[1] Hubei Polytechnic University, 4550573@qq.com

[2] Dalian University of Technology, lixin@dlut.edu.cn

[3] Hubei Polytechnic University, 107793168@qq.com

The random finite element method (RFEM) usually combines the random field theory and finite element method in the framework of direct Monte Carlo simulation (MCS) to perform slope reliability analysis with spatial variation of soil properties. However, the approach takes long time to calculate small failure probability (p_f) in the slopes. A new approach that combines subset simulation and the linked-list sifting method is proposed to calculate small p_f in the slopes, which consumes much less time than other approaches. In the proposed approach, soil properties are first transformed into discretized random fields. Next, the discretized random fields are used as input arguments in the linked-list sifting computer program to calculate the slope safety factors of initial sample points. Then, the conditional sample points are generated based on the initial sample points at different levels of subset simulation, which are used to determine the slope failure probability. Finally, a cohesive slope example is given to illustrate the effectiveness and efficiency of the proposed approach.

References

[1] Au, S. and Beck, J.L., 2001. Estimation of small failure probabilities in high dimensions by subset simulation. Probabilistic Engineering Mechanics, 16(4): 263-277.

[2] Cheng, Y.M., Lansivaara, T. and Wei, W.B., 2007. Two-dimensional slope stability analysis by limit equilibrium and strength reduction methods. Computers and Geotechnics, 34(3): 137-150.

[3] Fenton, G.A. and Vanmarcke, E.H., 1990. Simulation of random fields via local average subdivision. Journal of Engineering Mechanics, 116(8): 1733-1749.

[4] Griffiths, D.V. and Fenton, G.A., 2004. Probabilistic slope stability analysis by finite elements. Journal of Geotechnical and Geoenvironmental Engineering, 130(5): 507-518.

[5] Griffiths, D.V. and Lane, P.A., 1999. Slope stability analysis by finite elements. Geotechnique, 49(3): 387-403.

[6] Huang, J., Fenton, G., Griffiths, D.V., Li, D. and Zhou, C., 2016. On the efficient estimation of small failure probability in slopes. Landslides: 1-8.

[7] Li, D., Xiao, T., Cao, Z., Zhou, C. and Zhang, L., 2016. Enhancement of random finite element method in reliability analysis and risk assessment of soil slopes using Subset Simulation. Landslides, 13(2): 293-303.

[8] Li, H. and Cao, Z., 2016. Matlab codes of Subset Simulation for reliability analysis and structural optimization. Structural and Multidisciplinary Optimization: 1-20.

[9] Li, H. and Ma, Y., 2014. Discrete optimum design for truss structures by subset simulation algorithm. Journal of Aerospace Engineering, 28(4): 04014091.

[10] Luo, X., Cheng, T., Li, X. and Zhou, J., 2012. Slope safety factor search strategy for multiple sample points for reliability analysis. Engineering Geology, 129: 27-37.

[11] Song, S., Lu, Z. and Qiao, H., 2009. Subset simulation for structural reliability sensitivity analysis. Reliability Engineering & System Safety, 94(2): 658-665.

[12] Spanos, P.D. and Ghanem, R., 1989. Stochastic finite element expansion for random media. Journal of engineering mechanics, 115(5): 1035-1053.
[13] Tee, K.F., Khan, L.R. and Li, H., 2014. Application of subset simulation in reliability estimation of underground pipelines. Reliability Engineering & System Safety, 130: 125-131.
[14] Vanmarcke, E. and Grigoriu, M., 1983. Stochastic finite element analysis of simple beams. Journal of Engineering Mechanics, 109(5): 1203-1214.
[15] Vanmarcke, E., Shinozuka, M., Nakagiri, S., Schueller, G.I. and Grigoriu, M., 1986. Random fields and stochastic finite elements. Structural Safety, 3(3-4): 143-166.
[16] Zhang, J. and Ellingwood, B., 1994. Orthogonal series expansions of random fields in reliability analysis. Journal of Engineering Mechanics, 120(12): 2660-2677.
[17] Zhu, H., Zhang, L.M., Zhang, L.L. and Zhou, C.B., 2013. Two-dimensional probabilistic infiltration analysis with a spatially varying permeability function. Computers and Geotechnics, 48: 249-259.

Two-step computational homogenization of polymer nanocomposites considering particle agglomeration

Maenghyo Cho[1,*], Kyungmin Baek[2], Hyunseong Shin[3]

[1, 2, 3]Department of Mechanical and Aerospace Engineering, Seoul National University, Republic of Korea

[1]mhcho@snu.ac.kr, [2]myminvva@snu.ac.kr, [3]p2530@snu.ac.kr

Polymer nanocomposites have received a great deal of attentions over the past years and been applied in various industrial field due to their high level of thermal and mechanical properties. Nanoparticles in polymer composites often form agglomerations rather than form well-dispersed. Thus this agglomerations of nanoparticles imposes limitation in obtaining enhancement of thermo-mechanical properties reinforced by nanoparticles. As many researchers have conducted experiments and atomistic simulations to understand the effect of agglomeration, negative effects of agglomeration on the thermo-mechanical characteristics of nanocomposites have been reported. In our previous study, we quantified the elastic modulus of interphase near nanoparticles considering the degree of overlapping of interphase and confirmed that the increased size of agglomeration significantly decreases the homogenized elastic modulus of nanocomposites. Therefore, it is essential to understand the relation between the overall mechanical properties of nanocomposites and nanostructures including the various degree of agglomeration.

In this study, we investigated the effect of agglomeration on the mechanical behavior of nanocomposites using multiscale bridging methodology in which molecular dynamics (MD) simulation information is upscaled to the continuum micromechanics scale. We define a new index "Clustering density" which represents the degree of nanoparticulate agglomeration. We demonstrate this "Clustering density" mainly influences on the elastic modulus of nanocomposites. After domain decomposition of a large RVE, 1st homogenization analysis is conducted to obtain the homogenized elastic properties of the local subcell domain, as shown in Fig. 2. Specifically, 1st homogenization is proceeded 8 times in the present numerical example. In sequence, global homogenized properties of nanocomposites are obtained by the 2nd homogenization process. The proposed two-step computational homogenization anlaysis of polymer nanocomposites is compared to the direct numerical simulations (DNS) results to verify accuracy and effectiveness of the newly proposed model.

The new index "Clustering density (g)" is defined as below :

$$g = \mathrm{A}\left(1 - \frac{f_{fp} + \sum f_c}{f_{max}}\right) \tag{1}$$

Here, f_{fp} and f_c mean the volume fraction of free nanoparticle's interphase and agglomerated nanoparticle's interphase, respectively. f_{max} is the maximum volume fraction of interphase and A is normalization constants to make the range of clustering density from 0 to 1. Using the "Clustering density" index, we can predict the Young's modulus of nanocomposites as the following form :

$$E_{comp} = a \times e^{(-b \times g)} + c \text{ [GPa]} \tag{2}$$

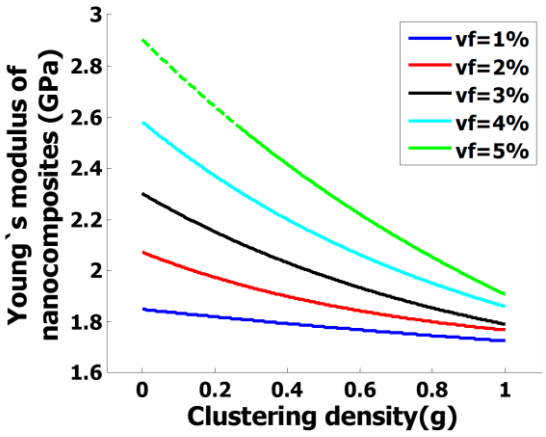


Figure 1. The elastic modulus of nanocomposites with different nanoparticle volume fraction

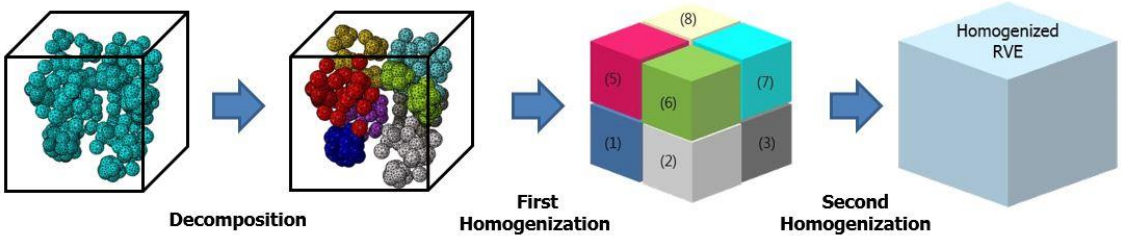


Figure 2. Schema of two step computational homogenization

Fig. 1. represents the mentioned exponent decay functions of the homogenized elastic modulus of nanocomposites including less than 50 nanoparticles. Fig. 2. describes the schematic process of two step computational homogenization .

We developed new two-step homogenization method combined with molecular dynamics simulations to analyze a large RVE embodying many nanoparticles. This model can handle nanoparticle agglomoration effect to predict elastic stiffness of homogenized RVE.

Acknowledgement

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

References

[1] Shin, H., Yang, S., Choi, J., Chang, S., Cho, M., 2015. Effect of interphase percolation on mechanical behaviour of nanoparticle-reinforced polymer nanocomposite with filler agglomeration : A multiscale approach. Chemical Physics Letter 635, 80-85.

[2] Shin, H., Baek, K., Han, J.-G., Cho, M., 2017. Homogenization analysis of polymeric nanocomposites containing nanoparticulate cluster. Composites Science and Technology 138, 217-224.

[3] Moore, J.A., Ma, R., Domel, A.G., Liu, W.K., 2014. An efficient multiscale model of damping properteis of filled elastomers with complex microstructures. Composites: Part B 62, 262-270.

FUTURE OF THE DISCRETE ELEMENT METHOD IN THE MODELLING OF THE GRINDING WHEEL

J.L. Osa[1,*], N. Ortega[2], G. Vidal[3], B. Fernandez-Gauna[4], A. Carballo[5]

[1]Mechanical Engineering Dpt., University of the Basque Country UPV/EHU, Eibar, Spain, j.osa@ehu.eus

[2] Mechanical Engineering Dpt., University of the Basque Country UPV/EHU, Bilbao, Spain, naiara.ortega@ehu.eus

[3]Mechanical Engineering Dpt., University of the Basque Country UPV/EHU, Bilbao, Spain, gorka.irusta@ehu.eus

[4]Computational Intelligence Group, University of the Basque Country UPV/EHU, Vitoria-Gasteiz, Spain, borja.fernandez@ehu.eus

[5]Desarrollos Mecánicos de Precisión S.L. (DMP), Mendaro, Spain, acarballo@dmp.aero

The method of sharpening tools in the bronze edge has been modified and largely improved, being nowadays the most popular process to finish high quality and precision mechanical components. Thus, unsurprisingly, the past 40 years the grinding process has been the target of an extensive research, especially by modelling and simulation. Grinding wheels are complex tools with a structure composed of abrasive grain material, a bonding material and pores. The undefined shaped grains do the cutting, whereas the bonding material provides cohesion to the ensemble. The grain distribution and combined stiffness define the performance of the tool, together with the surface topography created by dressing [1]. The ideal model would be the one that could combine the granular morphology of the grinding wheel, together with the stiffness arisen from the combined work of abrasive grits and binder.

Implicit numerical tools like the finite element method (FEM) could simulate the mechanical behaviour of a heterogeneous body. However, due to the size ratio between sharp grits and wheel, as well as the rounded porous network, the creation of an adequate extensive mesh. In addition, the adjustment of the constitutive relationships of the material would be demanding. The use of multi-scale modelling would decrease the size of the model. So far today, nobody has proposed a FEM model of the grinding wheel, but the geometrical description [2].

Recently, two models based on the discrete element method (DEM) have been presented to describe the mechanical behaviour of the grinding wheel [3, 4]. This explicit numerical tool tracks the movement of a huge amount of particles and it was initially developed for geotechnical purposes. DEM is able to describe naturally the random granular nature of the grinding wheel. The assumption of a single discrete element representing a single abrasive grit makes affordable the numerical description of the complex wheel structure. The bonds and interactions between elements bring stiffness to the whole, emerging the macro-mechanical properties of the wheel-body. The use of DEM in the modelling of the grinding wheels opens a range of possibilities in the simulation of the process.

The proposed paper aims to point out the promising path that will follow this novel research-line. In this work, a definition of the complex wheel structure is proposed in order to represent numerically and, in a great detail, the grinding wheel behaviour. After a brief state of the art related to the grinding wheel modelling, the ideal features that should comply such model are described. The characteristics that should be taken into account are the grain size, the grain geometry, the abrasive volumetric fraction and the wheel hardness. The meaning of the wheel hardness is the resistance to release a grit, which is indirectly evaluated by the elasticity. The bonds between discrete elements (spring or beam) determine the elasticity, and their properties have to be calibrated through homogenisation to match the macro-scale mechanical properties of the wheel.

The model of the grinding wheel is interesting in process optimisation and enhances the understanding in wear and deflection behaviour of the wheel.

References

[1] Malkin, S., Guo, C., 2008. Grinding technology: theory and application of machining with abrasives. Industrial Press Inc. New York, USA.

[2] Brakhage, K. H., Makowski, M., Klocke, F., Weiss, M., 2011. Grinding Wheel Modeling: Development of a mathematical Model. MASCOT11 Proceedings—IMACS Ser. Comput. Appl. Math.

[3] Li H., Yu T., Zhu L., Wang W., 2015. Modeling and simulation of grinding wheel by discrete element method and experimental validation. The International Journal of Advanced Manufacturing Technology, 1–18.

[4] Osa, J.L., Sánchez, J.A., Ortega, N., Iordanoff, I., Charles, J.L., 2016. Discrete-element modelling of the grinding contact length combining the wheel-body structure and the surface-topography models. International Journal of Machine Tools and Manufacture, 110, 43-54.

GLOBAL SENSITIVITY ANALYSIS OF REACTION KINETICS USING RATE RULES

M. Hantouche[1], M. Sarathy[2], O.M. Knio[3,*]

[1]PSE Division, King Adbullah University of Science and Technology, Thuwal, Saudi Arabia, mireille.hantouche@kaust.edu.sa

[2]PSE Division, King Adbullah University of Science and Technology, Thuwal, Saudi Arabia, mani.sarathy@kaust.edu.sa

[3]CEMSE Division, King Adbullah University of Science and Technology, Thuwal, Saudi Arabia, omar.knio@kaust.edu.sa

In this study, we investigate the sensitivity of the ignition delay time of n-butanol to uncertainties in kinetic rates parameters. This is commonly addressed using local, first-order sensitivity methods, which amount to characterizing the local variability due to small perturbations in a single (input) kinetic rate parameters. While these approaches can provide effective means of performing an initial screening of key parameters, they can suffer from substantial drawbacks. These include ignoring potentially important interactions between different uncertain inputs, i.e. mixed interactions, as well as inability to quantify overall variability in selected quantities of interest (QoIs).

In this work, we rely on a global sensitivity analysis (GSA) approach to overcome these drawbacks. The approach is based on first building a surrogate model of the QoIs. Polyomial chaos (PC) expansions are used for this purpose [1–3]. The unknown coefficients in the expansion are determined using an adaptive, pseudo-spectral projection technique [4]. This amounts to computing the QoIs on a sparse quadrature grid, which is anistropically refined in order to achieve a user-defined tolerance in the representation. By exploiting the orthogonality of the PC basis, variance-based first-order and total sensitivity indices can be readily determined that respectively characterize the direct and total contributions of individual input parameters to the total variance in the QoIs.

The GSA approach is applied to analyze the impact of uncertain rate parameters on the combustion of n-butanol in air, for different initial temperature, pressure conditions and different equivalence ratios. The detailed chemical kinetic model of [5], constructed utitlizing rate-rule concepts [6], is adapted to this end. Simply stated, rate rules is a systematic approach that estimates the rates of appreciably similar reactions to be the same. The n-butanol kinetic model used in this study comprises 30 reaction classes [5], which describe both low-temperature and high-temperature kinetic schemes for alcohol fuels. Assigned to each of these reaction classes is a uncertainty factor that characterizes the variability of the corresponding rate parameter.

The GSA is first applied to identify the rate rules whose uncertainties dominate the variability of the ignition delay time. Once these dominant parameters are identified, the GSA is exploited to reduce the dimensionality of the germ. Once unimportant rules are ignored, an additional layer of detail is introduced, namely by considering the impact of individual subrules belonging to the retained rules. As briefly illustrated below, this enables us to explore in a cost-effective fashion variability source at different levels.

We first consider a 30-dimensional stochastic germ in which each random variable is associated with one reaction class. A forward propagation of uncertainty is first used to propagate this uncertainty to the predicted QoIs. We find that the ignition delay time is mostly sensitive to variations in four major reaction classes, namely, H-atom abstraction from the fuel (reaction class 2), addition of O_2 to the fuel radicals (reaction class 11), fuel radical isomerization including Waddington type reaction mechanism (reaction class 15) and concerted eliminations reactions (reaction class 16). This result enables us to focus our attention on the four dominant reaction classes, and the validity of this restriction is ascertained by repeating the analysis for a four-dimensional germ, and verifying that the statistical properties of the ignition delay time are accurately captured using a the four-dimensional germ.

We then examine the subrules falling within these reaction classes. Reaction class 2 includes 11 subrules depending on the atom abstracting from the fuel. Hence, abstraction can occur by H, OH, O, O_2, HO_2, CH_3, HCO, CH_2OH, CH_3O, CH_3O_2 or C_2H_5. Reaction class 11 comprises of 3 subrules based on the abstraction site being primary, secondary or an α–site. Reaction class 15 includes 11 subrules determined by the transition state ring type (5, 6 or 7-membered), the nature of the C–H bond (primary, secondary, secondary with α–ROO or secondary β–ROO) and waddington reactions. Lastly, since it does not include any subclass, reaction class 16 is kept as one reaction class. We investigate the sensitivity of ignition delay time due to variability in the rate parameters of the 26 subrules at various stoichiometric conditions, initial temperatures in the range 700–1000K, and initial pressures in the range 20–80 bar. The global sensitivity analysis shows that at all the temperature and pressure conditions considered, uncertainties in HO_2 abstraction dominate the variability of the ignition delay time, even though abstraction by OH is the primary consumption pathway for the alcohol fuel. Additionally, at 700 and 800 K, the important subrules in reaction classes 11 and 15 are abstraction from the α–site and the α–ROO radical undergoing a 6-membered transition state ring isomerization at a secondary C–H bond site, respectively.

References

[1] Wiener, N., 1938. The homogeneous chaos. *American Journal of Mathematics*, *60*(4), pp.897-936.

[2] Ghanem, R.G. and Spanos, P.D., 2003. *Stochastic finite elements: a spectral approach*. Courier Corporation.

[3] Le Maître, O. and Knio, O.M., 2010. *Spectral methods for uncertainty quantification: with applications to computational fluid dynamics*. Springer Science & Business Media.

[4] Winokur, J., Kim, D., Bisetti, F., Le Maître, O.P. and Knio, O.M., 2016. Sparse pseudo spectral projection methods with directional adaptation for uncertainty quantification. *Journal of Scientific Computing*, *68*(2), pp.596-623.

[5] Sarathy, S.M., Oßwald, P., Hansen, N. and Kohse-Höinghaus, K., 2014. Alcohol combustion chemistry. *Progress in energy and Combustion Science*, *44*, pp.40-102.

[6] Westbrook, C.K. and Dryer, F.L., 1984. Chemical kinetic modeling of hydrocarbon combustion. *Progress in Energy and Combustion Science*, *10*(1), pp.1-57.

A Massively Parallel Localized Reduced Basis Multi-Scale Solver with EXA-DUNE and pyMOR

René Milk[1,*], Mario Ohlberger[1], Felix Schindler[1]

[1]Institute for Numerical and Applied Mathematics, University of Münster,{rene.milk,mario.ohlberger,felix.schindler}@wwu.de

The Mathematical models of complex flows, arising for example in reservoir engineering or water pollution dispersion prediction, are naturally of multi-scale and parametric character. They combine effects on multiple scales of space, ie. microscopic material features like porosity with macroscopic influences like external pressures or well placement. It is often impossible to know the exact material properties at every given point in the computational domain, but rather a statistical distribution needs to be assumed.

Our Localized Reduced Basis Multi-Scale Method (LRBMS) is especially well suited for the computational efficiency requirements arising from multi-query scenario like uncertainty quantification or optimization with its blending of accuracy enhancing multi-scale and parametric forward-solve accelerating reduced basis methods.

As a part of the German Science Foundation's Strategic Priority Programme 1648 “Software for Exascale Computing (SPPEXA)” project EXA-DUNE our goal is to develop a multi-level parallelization strategy for the LRBMS.

In this contribution we present strong and weak scaling benchmarks of our heterogeneous pyMOR/EXA-DUNE (Python/C++) software stack on a large scale supercomputer.

References

[1] Bastian, P., et al. "Advances concerning multiscale methods and uncertainty quantification in EXA-DUNE." Software for Exascale Computing-SPPEXA 2013-2015. Springer International Publishing, 2016. 25-43.

[2] Milk, R., Rave, S., Schindler, F. "pyMOR--Generic Algorithms and Interfaces for Model Order Reduction." SIAM Journal on Scientific Computing 38.5 (2016): S194-S216.

[3] Ohlberger, M., Schindler, F. "Error control for the localized reduced basis multiscale method with adaptive on-line enrichment." SIAM Journal on Scientific Computing 37.6 (2015): A2865-A2895.

ON THE INFLUENCE OF MECHANICAL PROPERTIES VARIABILITY IN THE ROBUSTNESS OF SHEET METAL FORMING PROCESSES

P.A. Prates[1,*], A.S. Adaixo, A.F.G. Pereira[1], M.C. Oliveira[1], J.V. Fernandes[1]

[1]CEMMPRE, Department of Mechanical Engineering, University of Coimbra, Pólo II, Rua Luís Reis Santos, Pinhal de Marrocos, 3030-788 Coimbra, Portugal, pedro.prates@dem.uc.pt, andreadaixo@gmail.com, andre.pereira@dem.uc.pt, marta.oliveira@dem.uc.pt, valdemar.fernandes@dem.uc.pt

The design and manufacture of high quality products with a minimum of costs requires robust design optimization techniques, developed to allow the determination of design solutions non-vulnerable to production tolerances, parameters drift, etc. [1]. In this context, the increasing competition within the aeronautical and automotive industries brings new challenges in the quality and robustness of the manufactured products. Robust design of sheet metal forming processes is a concept with special interest for Portuguese and European industry, since the aim is to reduce the scrap rate of this type of forming process.

Finite element analysis (FEA) is now a well-established computational tool in industry for understanding the mechanics of forming process and predicting the regions prone to the occurrence of defects. However, the optimisation of such processes is typically based on deterministic approaches, excluding the variability inherent to material properties, geometry and process parameters, which may have significant effects on the forming quality, leading to non-robust solutions. On the other hand, arbitrary confidence intervals are commonly used to integrate variability effects, which can lead to overly conservative or inconsistent designs of the sheet metal forming processes. Some authors integrated statistical descriptions of different sources of variability within FEA for screening the sensitivity of predictions to the selected parameters variability (e.g. [2, 3]). Coupling this sensitivity analysis with optimization and statistical metamodelling tools, such as the Response Surface Methodology (RSM), enables the definition of ranges for FEA input parameters (material, geometry and process) most likely to lead to the desired outputs, i.e. components without defects for an large operation window. In this context, due to the large number of parameters involved, One-Factor-at-a-Time (OFAT) and Design of Experiments (DOE) experiments are used for screening the most influent factors (i.e. input parameters) in a process [4], with the main purpose of simplifying the construction of metamodels by negleting the effect of the least relevant factors. However, the choice of the screening method and its statistical analysis have an impact on the number and type of factors identified as being relevant to a specific forming process, which directly affects the definition of the metamodels and the subsequent evaluation of the process robustness.

This work presents a numerical study on the influence of variability in the mechanical properties and initial thickness of metal sheets, in the springback and maximum thinning predicted for a sheet metal forming process. For this purpose, a mild steel alloy was selected as reference material and the U-rail drawing process was considered. The factors concerning the material properties selected for this study were: Young's modulus, E; Y_0, C and n of the Swift hardening law and the anisotropy coefficients r_0, r_{45} and r_{90} [5]. The stochastic variability of all factors was described by a probabilistic Gaussian distribution, with well defined mean and standard deviation values. Firstly, OFAT, Plackett-Burman

and 1/16 Fractional Factorial Design were tested for the screening design [6], performed using FEA results of the U-rail process, at two levels of blankholder force: 4.9 and 19.6 kN. Statistical analyses based on index of influence were performed for each screening design approach, to identify the most relevant factors, concerning the occurrence of springback and thinning in the forming process [2]. The comparison of the diferent screenning design approaches indicates that they can lead to simliar results, as shown in Figure 1, or to the selection of different factors, depending on the index of influence under analysis. This is also influenced by the approach selected to determine the most relevant factors. Then, RSM metamodels were built using Central Composite Designs [2], which allows establishing analytical relationships between the identified relevant factors and the responses (springback and thinning) and, consequently, evaluate the response variablity.

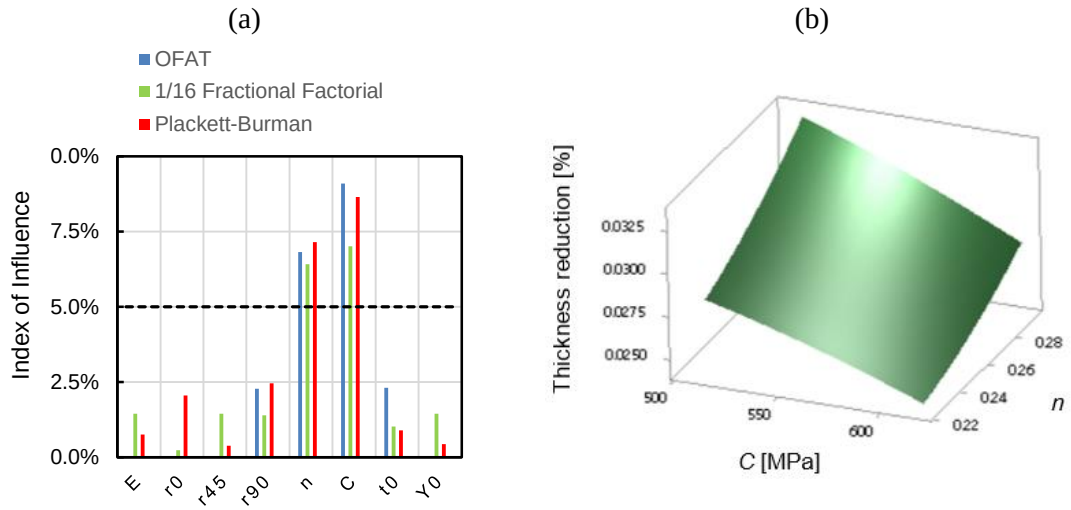


Figure 1. (a) Comparative screening analysis for maximum thinning with blankholder force equal to 4.9 kN: OFAT *vs.* Plackett-Burman *vs.* 1/16 Fractional Factorial designs. In all designs, the values of the indexes of influence obtained for the material parameters *n* and *C* are above the selected threshold of 5% (defined by the dashed black line), thus only *n* and *C* were considered for the definition of the RSM metamodel; (b) RSM metamodel establishing the analytical relationship between maximum thinning and *n* and *C* parameters.

References

[1] Beyer, H.G., Sendhoff, B., 2007. Robust Optimization – A Comprehensive Survey. Computer Methods in Applied Mechanics and Engineering 196, 3190–3218.

[2] Marretta, L., Di Lorenzo, R., 2010. Influence of Material Properties Variability on Springback and Thinning in Sheet Stamping Processes: a Stochastic Analysis. The International Journal of Advanced Manufacturing Technology 51, 117–134.

[3] Milesi, M., Logé, R.E., Pino Muñoz, D., Jansen, Y., Bouchard, P.-O., 2017. Accounting for material parameters scattering in rolled zinc formability. Journal of Materials Processing Tecnology 245, 134–148.

[4] Czitrom, V., 1999. One-Factor-at-a-Time versus Designed Experiments. The American Statistician 53, 126–131.

[5] Prates, P.A., Oliveira, M.C., Fernandes, J.V., 2016. Identification of material parameters for thin sheets from single biaxial tensile test using a sequential inverse identification strategy. International Journal of Material Forming 9, 547–571.

[6] Wass, J.A., 2010. First Steps in Experimental Design – The Screening Experiment. Journal of Validation Technology 16, 49–57.

A Macro-Scale Topology Optimization Method for Flow through Arrays of Solid Structures

Geert Buckinx[1,2,*], Martine Baelmans[3]

[1]KU Leuven, Department of Mechanical Engineering, Celestijnenlaan 300A, 3001 Leuven, Belgium; [*]geert.buckinx@kuleuven.be

[2]EnergyVille, 3600 Genk, Belgium

[3]KU Leuven, Department of Mechanical Engineering, Celestijnenlaan 300A, 3001 Leuven, Belgium

Compact heat transfer devices like microchannel heat sinks and micro heat exchangers, as well as microreactors and other microfluidic devices often contain fluid flow systems consisting of spatially periodic solid structures. These spatially periodic solid structures appear as fin or tube arrays for instance, with the purpose of enhancing the performance and compactness of the device.

However, such spatially periodic solid structures usually do not result in an optimal design. The performance and compactness of a fluid flow system can be significantly improved by optimizing the lay-out and shape of its solid material through topology optimization [1-4]. The solid material then does no longer have to be distributed in the form of spatially periodic structures. Instead, the topology, i.e. the material distribution of fluid and solid, is determined by an optimization algorithm.

The current topology optimization methods for fluid flow systems are nearly all based on direct numerical simulation (DNS) of the flow equations. Therefore, they require to resolve the flow field on a very fine mesh when the flow features change over a length scale much smaller than the overall length scale of the flow system. Since the flow systems that emerge from topology optimization typically consist of (tree-like) branched channels with small-scale solid structures in between [5,6], the need for a fine mesh is the rule rather than the exception. Unfortunately, the required mesh fineness often leads to a huge computational cost, making topology optimization methods based on DNS infeasible for the practical design of many flow systems.

A second problem is that the current topology optimization methods frequently yield flow system designs which are too difficult to manufacture. Complex topologies with many degrees of freedom like branched channels with small-scale solid structures in between are in general more difficult to manufacture than arrays of spatially periodic solid structures.

To circumvent the former two problems, we present a macro-scale topology optimization method for flow systems consisting of an array of solid structures with a fixed shape and position, but with a varying size. By optimizing the size of each solid structure, the method allows us to maximize the hydraulic performance of the flow system for a desired material volume, hence compactness. As the minimal and maximum size of each solid structure are taken into account as design constraints, the manufacturability of the optimized design can be ensured.

Instead of relying on DNS, the presented method relies on solving the spatially filtered Navier-Stokes flow equations [7] to obtain the macro-scale flow field through the array of solid structures. The macro-scale flow field contains only the average flow features

occuring over a length scale larger than the characteristic size of a single solid structure. The detailed flow features occuring over smaller length scales are not resolved, but their effect on the macro-scale flow is modelled via an interfacial force. That way, our approach requires a much coarser mesh than DNS.

The macro-scale topology optimization method is applied to a flow system composed of solid cylindrical tubes. In order to optimize the diameter of each solid cylinder, the interfacial force is approximated from the Ergun equation [8]. The results of our method are compared to a pipe bend problem similar to that of Borvall et al. [1].

References

[1] Borrvall, T., Petersson, J., 2003. Topology optimization of fluids in Stokes flow. International Journal for Numerical Methods in Fluids 41, 77-107

[2] Guest, J. K., Prévost, J. H., 2006. Topology optimization of creeping fluid flows using a Darcy-Stokes finite element, International Journal for Numerical Methods in Engineering 66, 461-484

[3] Zhou, S., Li, Q., 2008. A variational level set method for the topology optimization of steady-state Navier–Stokes flow, Journal of Computational Physics 227, 10178– 10195

[4] Deng, Y., Liu, Z., Zhang, P., Liu, Y., Wu, Y., 2011. Topology optimization of unsteady incompressible Navier–Stokes flows, Journal of Computational Physics 230, 6688-6708

[5] Marck, G., Nemer, M., Harion, J. L., 2013. Topology optimization of heat and mass transfer problems: laminar flow, Numerical Heat Transfer, Part B: Fundamentals: An International Journal of Computation and Methodology 63, 508-539

[6] Koga, A. A., Lopes, E. C., Villa Nova, H. F., de Lima, C. R., Nelli Silva, E. C., 2013. Development of heat sink device by using topology optimization, International Journal of Heat and Mass Transfer 64, 759-772

[7] Buckinx, G., Baelmans, M., 2015. Multi-scale modelling of flow in periodic solid structures through spatial averaging. Journal of Computational Physics, 291, 34-51.

[8] Ergun, S., 1952. Fluid flow through packed columns. Chemical Engineering Progress, 48, 89-94.

THE MODEL-BASED MULTIOBJECTIVE OPTIMIZATION OF CURE PROCESS CONTROL FOR A LARGE CFRP POLYMERIC COMPOSITE PANEL

Sergey Shevtsov[1,*], Ilya Tarasov[2], Jiing-Kae Wu[3] and Igor Zhilyaev[1]

[1]South Center of Russian Academy, Rostov on Don, Russia, sergnshevtsov@gmail.com

[2] AP Group – Carbon Studio, Saint-Petersburg, Russia, ilya.tarasov@carbonstudio.ru

[3]National Kaohsiung Marine University, Kaohsiung City, Taiwan R.O.C., jiingkae.wu@gmail.com

A wide variety of composite components that has the open-shell geometry or smooth panel shape, are widespread in aircraft structures. The open-mould forming technology, which is the most suitable for components with such geometry, use of only one mould surface, over which the layers of reinforcing fibres or fabric are tightly placed. Then a mould packed with a raw material is placed into a vacuum bag made of a flexible plastic film embracing the surface of the lay-up, and a vacuum-tight bag together with a mould is disposed in an autoclave [1, 2]. The first stage of this cure cycle consists of increasing the temperature at a controlled rate up to the start of resin fluidization and dwelling at this temperature until the minimum resin viscosity is reached. Such an isothermal hold is applied at the stages of resin fluidization as well as at the process completion to allow the temperature distribution to become more uniform, especially in large components with thickness variations. At the end of cure cycle after resin vitrification, the temperature is slowly reduced while the laminate is still under pressure. The trial-and-error approach to the tooling design and cure process development that causes the high cost of advanced composites, especially for the large composite structures can be overcome by the use of process modelling or simulation that can predict a desired tooling and process design window. Such a process model should correctly describe a number of coupled physical and chemical phenomena, including heat transfer, thermal, kinetic and rheological properties of material transformation during cure parts of complex shape, and should take into account different constraints imposed by the process equipment, material properties, etc.

We present the model-based technique and results of the cure process optimization of large CFRP panel with dimensions ~20*2.5 m, thickness 4…8 mm, which has a number of longitudinal reinforcing stringers. Our study consisted of the following phases. In order to determine the thermal and kinetic properties of the used prepreg the dynamic DSC tests have been carried out using NETZSCH equipment at the heating rates 0.8…1.5 deg/min. On the base of DSC study all six parameters of autocatalytic equation

$$\partial\alpha/dt = \left[A_1 \exp\left(-\frac{E_1}{RT} \right) + A_2 \exp\left(-\frac{E_2}{RT} \right) \cdot \alpha^m \right] (1-\alpha)^n , \qquad (1)$$

which adequately describes resin cure at the varying heating rate, have been identified using numerical technique of evolutionary computing. In Eq.1 degree of cure α is defined by the relationship $Q_{exo} = Q_{tot} \cdot \partial\alpha/\partial t$ between actual value of exothermal heat Q_{exo} and enthalpy Q_{tot} of cure reaction; E_1, E_2 are the activation energies, R is the universal gas constant, T is the Calvin temperature, m, n are the reaction orders, and t is time. As the further results of kinetic model identification the enthalpy Q_{tot} =0.105 MJ/kg of cure reaction and dependence of specific heat capacity (in J/(kg•K)) on degree of cure were found

$$C_p = 2300 - 550 \cdot \alpha . \qquad (2)$$

DEA testing results of the prepreg that describe the transformation of the resin rheology during cure then have been analyzed to determine the temperatures of both isothermal holds. Geometry

of the cured part together with a mould made of thick-walled CFRP has been redesigned to exclude some topological imperfection, and exported to the finite element soft package. The forward cure modeling system for the prepreg cure consists of coupled heat transfer

$$\rho_{c/m} C_{c/m} \partial T / \partial t + \nabla \cdot \left(- k_{c/m} \nabla T \right) = \begin{cases} Q_{exo} \\ 0 \end{cases} \qquad (3)$$

and kinetic equations (1), whose coefficients depend on the temperature and degree of cure.

To facilitate the finite element meshing the thermal resistance and thus the presence of the vacuum bag thin film were neglected, whereas release film separating prepreg and upper surface of mould was substituted by the special boundary condition

$$-\mathbf{n}_d \cdot \left(-k \left(\nabla_t T_s + \nabla_n T_s \right) \right) = -\left(T_u - T_d \right) / R_s ; \quad -\mathbf{n}_u \cdot \left(-k \left(\nabla_t T_s + \nabla_n T_s \right) \right) = -\left(T_d - T_u \right) / R_s , \qquad (4)$$

where

$$R_s = -d_s / k ; \quad T_u = T_s \mid_{L=0} ; \quad T_d = T_s \mid_{L=d_s} , \qquad (5)$$

$\mathbf{n}_u$ and $\mathbf{n}_d$ are the normal vectors to the upper and lower boundaries of the film layer, d_s is the film thickness, and T_s is the auxiliary variable, which is determined inside virtual layer only.

In order to find an appropriate finite element meshing and indicative values of the time integration step, several segments were cut from a while panel (see Fig. 1). All boundary conditions corresponded to the two-stages heating in autoclave.

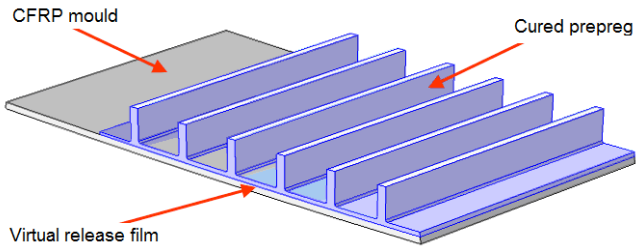


Figure 8. An example of segment that was cut from a whole panel for the preliminary testing FEM model.

The results of these preliminary simulations then have been used at the finite element implementation of forward problem of whole panel curing process in Comsol Multiphysics 5.2 environment. For the whole FEM model of the cured panel the numbers of degree of freedom are for the heat transfer subtask 303,758 and for the thermal kinetic one 232,584. Computation time for one set of the design variables using distributed FEM solver and 4-core I7 computer is 1.5 hrs.

Assuming a two-stage cure cycle, we varied the duration of the first and second heating up and also the duration of two dwelling sections to provide the minimum objectives: averaged variations of the cure degree and temperature gradient, which were calculated by integration within the cured part. The maximum durations of each cure stage, the whole cure cycle and temperatures at the first and second isothermal holds are constrained. Optimum area in a four-dimensional design space has been visualized by the set of its two-dimensional projections with the contour lines that determine the values of the objectives.

The suggested approach allows understanding the complex nature of curing phenomena in a large composite part with complex geometry, measuring the maximum achievable process quality, finding values satisfying the constraints imposed by the control law parameters, and making a reasonable decision on the choice of such values.

Uncertainty Quantification with discontinuous Galerkin discretization for Aeroacoustic applications

Thomas Kuhn[1,*], Jakob Duerrwaechter[1], Fabian Meyer[2]

Dr. Andrea Beck[1], Prof. Claus-Dieter Munz[1], Prof. Christian Rhode[2]

[1]Institute of Aerodynamics and Gas Dynamics, University of Stuttgart

[2]Institute of Applied Analysis and Numerical Simulation, University of Stuttgart

The direct numerical computation of acoustic noise (Direct Noise Computation, DNC) generated by fluid flows offers a number of advantages compared to a hybrid approach, in which both fields are solved independently. In DNC, hydrodynamics and acoustics are solved in a coupled manner which allows the detection and numerical representation of intricate interactions between both fields, e.g. feedback loops which generate tonal noise [1]. However, this approach intrinsically requires the resolution of the disparate length and time-scales of non-linear turbulent production and the acoustic propagation, making DNC a challenging example of a multiscale problem.

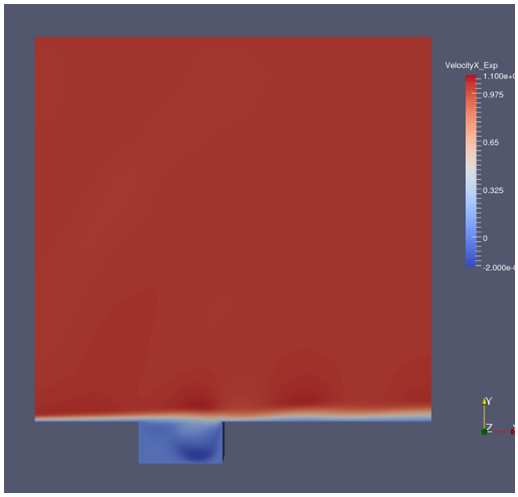
In recent years, high order Discontinuous Galerkin (DG) methods have gained significant attention as baseline schemes for multiscale problems. Due to low numerical approximation errors, geometric flexibility and excellent high performance computing capabilities, they have been successfully applied to large multiscale simulations. An open-source framework based on a computationally efficient variant of the DG method has been developed by the Numerics Research group and has been successfully applied to DNS and LES of turbulent flows [2, 3]. In particular, this framework has proven its capabilities for DNC in predicting acoustic feedback loops in complex geometries [1]. However, due to the strong non-linear processes involved, the occurrence of acoustic feedback phenomena are highly sensitive to turbulence, geometry details and the quality of the numerical scheme and its generation is still not fully understood. Therefore, our aim is to develop an uncertainty quantification (UQ) framework based on the existing deterministic flow solver to examine the influence of uncertain factors.

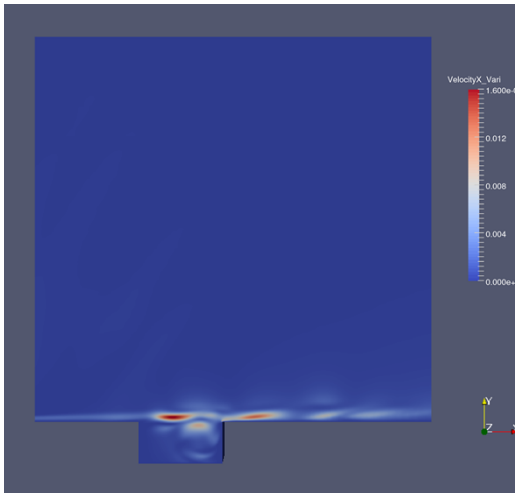
In a first step, we focus on non-intrusive methods, while an approach based on a stochastic Galerkin expansion of the solution will follow later. Among the non-intrusive approaches, we have implemented an efficient variant of the Monte Carlo (MC) method. In this multi-level MC approach, different levels of spatial discretization of the same deterministic problem with random initial or boundary conditions are generated. The total number of sample computations is then distributed among these levels, with most of the computations being conducted on the cheapest, i.e. coarsest level. The basic idea is to capture stochastic moments with a high stochastic resolution on the coarse levels, and to correct them with evaluations on the finer grids. In this talk, we will present this framework and its coupling to the high performance DG code and discuss the influence of the chosen sample number estimators on overall efficiency.

This framework will be applied to a 2D open cavity flow problem in which an acoustic feedback mechanism evolves. While in this configuration, the prediction of the frequencies of the feedback loop is well understood, the sound pressure level of this tonal noise is highly sensitive to uncertain geometry and various flow parameters. In our investigations, we will introduce uncertainties into the geometric configuration (cavity aspect ratio, downstream edge shape) and flow parameters. At the conference, we will

discuss the sensitivity of the hydrodynamics and pressure spectra with respect to the uncertain input. For example in a preliminary study we have chosen an uncertain viscosity in a 2D open cavity MLMC simulation. Results of the expectation and variance of the u velocity component are given in the figures below.

Finally we will present the convergence behavior of the sample distribution estimator. This framework will serve as a baseline for future developments. We plan to include gPC methods as well as develop an intrusive SG approach.





References

[1] Frank, H.M., Munz, C.-D., 2016. Direct aeroacoustic simulation of acoustic feedback phenomena on a side-view mirror. Vol 371: Journal of Sound and Vibration.

[2] Beck, A.D., Bolemann, T., Flad, D. et al., 2014. High-order discontinuous Galerkin spectral element methods for transitional and turbulent flow simulations. Vol 76: International Journal for Numerical Methods in Fluids.

[3] Atak, M., Larsson, J., Gassner, G., Munz, C.-D., 2014. DNS of a flat-plate supersonic boundary layer using the discontinuous Galerkin spectral element method. 44th AIAA Fluid Dynamics Conference.

NUMERICAL QUANTIFICATION OF SPATIAL VARIABILITY IN TOW REINFORCEMENT GEOMETRY OF CARBON COMPOSITE MATERIALS

D. Vandepitte[1,*], A. Vanaerschot[2], I. Straumit[3], S.V. Lomov[3]

[1]KU Leuven, Mechanical Engineering Department, dirk.vandepitte@kuleuven.be

[2]Brussels Airlines, andy.vanaerschot@brusselsairlines.com

[3]KU Leuven, Materials Engineering Department, straumit.ilya@kuleuven.be, stepan.lomov@kuleuven.be

Oberkampf et al. [1] have developed a comprehensive nomenclature to describe the nature of non-determinism as it occurs in design and verification procedures in modern engineering reality when developing advanced structures. In the assumption that the model and the numerical procedures which are used are correct, non-determinism is considered on model parameters only. They distinguish between on the one hand epistemic uncertainty, also simply called uncertainty, when knowledge is insufficient or information is incomplete, and on the other hand aleatory uncertainty, also called variability, when system characteristics vary from one realisation to another one or from one condition of utilisation to another. Different numerical formalisms are proposed to handle both categories [2]. Conditions of epistemic uncertainty with insufficient information require a non-probabilistic approach, either using interval arithmetic or with fuzzy analysis. Conditions of aleatory uncertainty occur when scatter on model parameters over different realisations is well quantified, in all aspects, including correlation between different model parameters, and in such case probabilistic analysis is viable. Probabilistic approaches are obviously preferred as they allow for statistical interpretation of the result, such as probability of failure. It is observed however that many engineering practitioners, both in the scientific community and in industry, consciously or unconsciously adopt a probabilistic procedure although probability density functions (pdf) are not fully validated and complemented with subjective data, such as assumptions on the nature of the pdfs, on the magnitude of the coefficients of variation or on cross-correlations between different model parameters. Results are then unreliable.

Composite materials have been developed as lightweight solutions for demanding structural applications. There are many types of fibre reinforcements, in a uni-directional arrangement, in weaves, braids, knits, ... Not only the structure is designed but also the material needs to be designed for a specific application, paying attention to a wide range of criteria, which are often related to each other. Not only the structural strength and stiffness need to be verified, also the appropriate production process must be selected. This involves a wide range of design parameters. Typical applications like aircraft structures, automotive structures, sports goods, ... are usually subject to very strict performance requirements, implying that uncertainty and scatter need to be taken into account in the analysis and qualification processes. Scatter occurs at different levels of the composite material, inside the representative volume element (RVE) and also over a range of several RVEs.

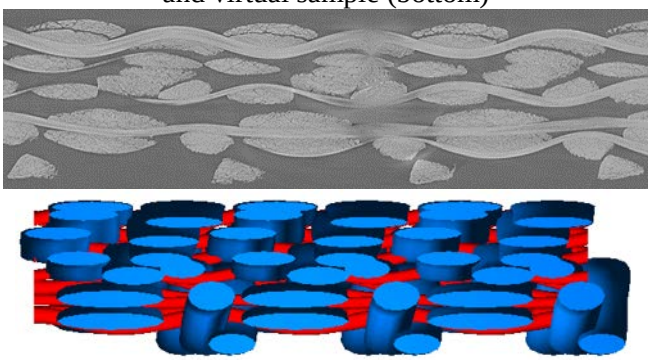
Schuëller et al. [3] call upon material scientists to establish a validated data base for a realistic representation of such a complex, multi-parameter system. This paper presents the general approach and successive steps to build random virtual specimens, which are subsequently used to evaluate the spatial variation in a carbon fibre reinforced 2/2 twill weave. The paper focusses on the quantification of variability in the geometrical representation of the fibre reinforcement architecture, with a particular focus on warp and

weft tow paths, tow cross-sections and their aspect ratios. A correct representation of the materials geometry and properties can only be achieved by (i) collecting enough experimental data on the spatially correlated random fluctuations of uncertain tow path parameters and (ii) deriving probabilistic information for the macroscopic properties from the lower scale mechanical characteristics.

Experimental data are collected of the random geometrical structure of the woven textile composite. Tow path properties are analysed on the short- and long-range, i.e. spanning several unit cells. The spatial variation of each tow parameter is decomposed in non-stochastic, periodic systematic trends and non-periodic stochastic fluctuations. The systematic trend represents the average behaviour of the tow parameter, while the stochastic characteristics are given in terms of the standard deviation and correlation length. Cross-correlations are taken into account, a cross-correlated series expansion is used, based on a Karhunen-Loève decomposition, as proposed by Vorechovskỳ [4]. In the final step, WiseTex models are generated. WiseTex [5] is a pre-processor for the generation of virtual 3D models of textile composites. The pre-processor prepares for the generation of finite element models for the mechanical analysis of composite structures. The statistics of the virtual models which are generated match all statistical characteristics of the hardware samples, both in short range and in long range.

The procedure is applied to a carbon fibre reinforcement system with a complicated architecture. Figure 1 shows the µCT image of the cross-section (top) and a WiseTex model of one of the samples which is generated (bottom). Statistics of the full set of the generated samples match the statistics of the experimental data set.

Figure 1: cross-section of the carbon fibre reinforced material in warp direction: µCT scan (top) and virtual sample (bottom)



References

[1] Oberkampf W., DeLand S., Rutherford B., Diegert K., Alvin K., A new methodology for the estimation of total uncertainty in computational simulation, Proceedings of the 40th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference, AIAA-99-1612:3061-3083, 1999

[2] Moens D., Vandepitte D.: A survey of non-probabilistic uncertainty treatment in finite element analysis, Computer Methods in Applied Mechanics and Engineering, 194 (14-16):1527-1555, 2005

[3] Charmpis D.C., Schuëller G.I., Pellissetti M.F., The need for linking micromechanics of materials with stochastic finite elements: a challenge for materials science, Computational Materials Science, 41(1):27-37, 2007

[4] M. Vorechovský, D. Novák, Correlation control in small-sample Monte Carlo type simulations 1: A simulated annealing approach, Probabilistic Engineering Mechanics, 24(3):452-462, 2009

[5] http://www.mtm.kuleuven.be/Onderzoek/Composites/software/wisetex, 2015

INTERVAL FINITE ELEMENT ANALYSIS OF COMPOSITE LAMINATES WITH SPATIALLY VARYING UNCERTAINTIES USING ABAQUS

Eugenia Romeo[1,*], Olga Barrera[2], Alba Sofi[3]

[1]Department of Civil, Energy, Environmental and Materials Engineering, University "Mediterranea" of Reggio Calabria, eugenia.romeo@unirc.it

[2]Department of Engineering Science, University of Oxford, olga.barrera@eng.ox.ac.uk

[3]Department of Architecture and Territory, University "Mediterranea" of Reggio Calabria, alba.sofi@unirc.it

Multilayer fibre-reinforced composite structures are conceived as a complex design arranging fibres and matrix properties. In order to model their behaviour, a number of material parameters, which may not be known deterministically, need to be taken into account. This is the main reason why, over the last decades, extensive research has been devoted to the development of non-deterministic models to describe the uncertain input parameters. In this context, recently, several non-probabilistic approaches have gained popularity as alternative tools for modeling uncertainties when experimental data are not sufficient to define the Probability Density Function requested by classical probabilistic methods. In this framework, the interval model [1] has proved to be a very useful tool when only information on the range of variability of the uncertain properties is available. Moreover, the sources of uncertainty exhibit significant spatial variabilities, from a macro-mechanical point of view, due to the variations in the individual lamina properties.

The aim of this study is to formulate an Interval Finite Element Method (IFEM) for the static analysis of laminated composite structures and to implement it into the commercial software ABAQUS. In order to take into account their intrinsic spatial variability, uncertainties are described by using the interval field model [2], recently introduced in the literature as a natural extension of the random field concept, based on the so-called Improved Interval Analysis (IIA) [3].

The bounds of the interval static response of composite structures with uncertain properties modeled as interval fields are evaluated through a Response Surface approach [4], which requires a certain number of deterministic analyses at selected sampling points. Such analyses are efficiently performed within the ABAQUS software framework, taking advantage of the User Material (UMAT) subroutines, coded in FORTRAN language. In order to demonstrate the efficiency of the proposed IFEM, numerical results concerning composite structures with uncertain lamina properties and an example of three point bending test validated experimentally are included. For validation purpose, appropriate comparisons with the exact bounds of the interval response provided by a time-consuming combinatorial procedure, known as vertex method [5], are carried out.

One of the main advantages of the proposed IFEM is that the analysis of complex composite structures with spatially varying interval properties can be efficiently performed by exploiting the potential of the commercial FE software ABAQUS.

References

[1] Moore, R.E., Kearfott, R.B., Cloud, M.J, 2009. Introduction to interval analysis. SIAM, Philadelphia.

[2] Verhaeghe, W., Desmet, W., Vandepitte, D., Moens, D., 2013. Interval fields to represent uncertainty on the output side of a static FE analysis. Computer Methods in Applied Mechanics and Engineering 260, 50-62.

[3] Muscolino, G., Sofi, A., Zingales, M.,2013. One-dimensional heterogeneous solids with uncertain elastic modulus in presence of long-range interactions: interval versus stochastic analysis. Computers and Structures 122, 217-229.

[4] Bucher, C., 2009. Computational analysis of randomness in structural mechanics. Ed. by D. M. Frangopol. Structures and Infrastructures Book Series, Vol. 3. Taylor & Francis, London.

[5] Dong, W., Shah, H., 1987. Vertex method for computing functions of fuzzy variables. Fuzzy Sets Syst 24, 65‑78.

FUZZY SET MEMBERSHIP FUNCTION DEFINED BY A MATERIAL MODEL RESPONSE AND USED IN UNCERTAINTY QUANTIFICATION

Jan Chleboun[1,*], Ielizaveta Kholmetska[2], Pavel Krejčí[3]

[1]Faculty of Civil Engineering, Czech Technical University in Prague, jan.chleboun@cvut

[2]Faculty of Civil Engineering, Czech Technical University in Prague, ielizaveta.kholmetska@fsv.cvut.cz

[3]Institute of Mathematics, Academy of Sciences of the Czech Republic, krejci@math.cas.cz

In [1], a mathematical model of a magnetostrictive energy harvester was proposed. In essence, the harvester consists of a Galfenol rod forming the core of a coil that is immersed in a bias magnetic field. If a periodic mechanical stress is applied to the Galfenol specimen, an electric current is produced in the coil. To describe the hysteresis of the material, the original harvester model [1] exploits the Preisach operator defined by means of a density function identified from measurements [1,2]. The use of the Preisach operator slows down the computations, especially if the harvester model serves as a state equation that is repeatedly solved in an optimization loop or in an uncertainty quantification problem.

Since the amount of hysteresis is small in Galfenol [2], a simplified, non-hysteretic material model was developed and its parameters identified in [3]. The material model outputs satisfactorily correspond to the values obtained by measurements. The harvester model is then represented by a nonlinear differential equation without the Preisach operator.

The fundamental parameter of the material model is g, a function of one variable that appears in the expression for the magnetization curve as well as for the magneto-elastic curve and that is considered uncertain. The uncertainty is modeled by a fuzzy set G, that is, by an admissible set of crisp functions that is fuzzified by a membership function.

Unlike the common approach to uncertain functions where the membership function value is based on a norm of the direct difference between an admissible function and a given function associated with the possibility degree one, a model-based fuzzification is applied. The membership function value is determined by the difference between the material model magnetic and magneto-elastic response and the measured Galfenol magnetic and magneto-elastic curves. In detail, the function g that minimizes the least squares difference between the material model response and the measurements has the possibility degree one. If the minimum least squares difference is relaxed by a parameter α, then parameters g belonging to an α-dependent set are allowed to represent the material model and, as a consequence, to determine the output of the energy harvester model. The α-dependent range of the harvested energy defines an α-level cut of the fuzzy harvester output.

The membership function of the harvester output is calculated by solving worst- and best-case energy harvesting scenario problems defined on a sequence of α-level subsets of the admissible set G that are determined by α-dependent bounds on magnetic and magneto-elastic response of the material model.

Although this approach is computationally more demanding than the norm-based fuzzification, it is more natural because it links together the available information (measurements) and the material model response to assess the uncertainty in the energy harvester model output.

Acknowledgement: This research has been financially supported by the Czech Science Foundation under Grant No. 15-12227S.

References

[1] Davino, D., Krejčí, P., Pimenov, A., Rachinskii, D., Visone, C., 2016. Analysis of an operator-differential model for magnetostrictive energy harvesting. Communications in Nonlinear Science and Numerical Simulation 39, 504–519.

[2] Davino, D., Krejčí, P., Visone, C., 2013. Fully coupled modeling of magneto-mechanical hysteresis through 'thermodynamic' compatibility. Smart Materials and Structures 22, 095009.

[3] Kholmetska, I., Chleboun, J., Krejčí, P. Numerical modeling of Galfenol magnetostrictive response. Submitted to Applied Mathematics and Computation.

NON-LOCAL HYDRODYNAMIC MESOSCALE MODEL IN SLIT NANOPORES

Diego Camargo-Trillos[1], J.A. de la Torre[2], Pep Español[2], Rafael Delgado-Buscalioni[3], Farid Chejne-Janna[1]

1 Facultad de Minas,Universidad Nacional de Colombia, Medellín, Colombia

2 Dept. Física Fundamental, Universidad Nacional de Educación a Distancia, Madrid, Spain

3 Universidad Autónoma de Madrid, Madrid Spain

We have derived from first principles the equations of hydrodynamics near a solid wall, valid for the study of the nanoscale. We generalize Dynamic Density Functional Theory (**DDFT**) by including not only the mass density field as in usual approaches to **DDFT**, but also the momentum density field of the fluid. In this new theory, the fluid moves according to a set of *non-local* hydrodynamic equations that include explicitly the forces due to the solid. These forces are of two types, reversible forces emerging from the free energy density functional, and accounting for impenetrability, and irreversible forces that involve the velocity of both the fluid and the solid. These forces are localized in the vicinity of the solid surface. The non-locality of the equations is due to the non-locality of the transport coefficients, which are given explicitly in terms of Green-Kubo formulae.

We particularize this general hydrodynamic **DDFT** for simple fluids to the case of slit nanopores with planar flow configurations. In this simple geometry, only a reduced number of non-local transport coefficients (**wall friction**, **slip friction**, and **viscous friction**) are needed in this planar configuration. The continuum hydrodynamic equations for a fluid in a slit nanopore are discretized into bins. This allows us both, to compute explicitly the Green-Kubo expressions for the non-local transport coefficients, and to solve numerically the continuum hydrodynamic equations.

The Green-Kubo formulae are computed from the time correlations of the force density , and the stress tensor of each bin. The phase functions trajectories are obtained from extensive Equilibrium Molecular Simulations of a slit nanopore with 10nm(length between planar walls) for a fluid reduced density of 0.24, 0.61, and 0.81. The non-local transport show the high space correlation of the **slip friction** coefficient at a density function. These Green-Kubo transport coefficients are subsequently used for the explicit numerical solution of the discrete hydrodynamic equations. A initial non-equilibrium profiles of the **plug** flow form are allowed to decay towards equilibrium. Non-Equilibrium Molecular Dynamics simulations and the predicted flow from the discrete hydrodynamic equation are then compared, with excellent agreement, with a complete prediction of the slip velocity of the system.

A MODEL FOR MASS TRANSPORT IN POROUS MEDIA BASED ON A HYBRID PROBABILISTIC/DETERMINISTIC APPROACH

López, E.A.[1,*], Mejía, J.M.[2], Chejne, F.[3]

[1]Universidad Nacional de Colombia – Universidad de Antioquia, ealopez@unal.edu.co

[2]Universidad Nacional de Colombia, jmmejiaca@unal.edu.co

[3]Universidad Nacional de Colombia, fchejne@unal.edu.co

A hybrid model based on a probabilistic approach [1], [2] and an Eulerian model [3], [4], was developed to study the multiphase flow and multicomponent transport in porous materials. The Eulerian model describes the multiphase flow using mass balance equations of each phase at the representative elemental volume (REV) scale. In the probabilistic approach, an evolution equation of the probability density function (PDF) of a transported scalar is developed, accounting for non-equilibrium mass transfer phenomena, a Fokker Plank - type equation. The aim of this paper is to extend the general framework for this alternative modeling approach to α-components, accounting for non-equilibrium mass transfer phenomena such as dissolution, diffusion and adsorption/desorption [5], [6].

The Eulerian model is discretized with the finite volume method (FVM). The numerical solution of the resulting non-linear set of equations provides pressures and saturations evolution for each grid block [3].

On the other hand, the PDF equation is solved using the Lagrangian stochastic particle method (SPM) [7], [8]. The SPM is based on a set of stochastic particles accounting for the mass of the phase it belongs to. Each stochastic particle represents the mass components of each phase in the porous medium [7], such as hydrocarbons, nanoparticles, polymers, surfactants, among other scalars. Here each particle may have associated one o several scalar properties, e.g., mass, concentration [7],[9], temperature [10], etc.

The deterministic and probabilistic approaches are coupled as follows: phases velocities are calculated from pressure and saturation fields (deterministic) and further transferred to the SPM. Velocity is used to do advance particles in the physical space. Then, particles are evolved in the compositional space and their composition is used for estimating mass transport properties (diffusion and dispersion coefficients), mass transfer models coefficients thermodynamic, and thermodynamic properties. These properties are transferred to the FVM solver where pressure and saturations are reevaluated. The process is repeated until the convergence criterion be fulfilled, for each time step.

Various one and two-dimensional numerical experiments demonstrate that with appropriate stochastic rules the particle solutions are consistent with a standard two-phase Darcy flow formulation [7].

References

[1] S. Pope, “PDF Methods For Turbulent Reactive FLows,” *Progress in Energy and Combustion Science*, vol. 11, no. 1. Pergamon Press Ltd., pp. 119–192, 1985.

[2] S. B. Pope, “Lagrangian PDF Methods for Turbulent Flows,” *Annu. Rev. Fluid Mech.*, vol. 26, no. 1, pp. 23–63, 1994.

[3] J. Bear, *Dynamics of Fluids in Porous Media*, First Edit. New York: Dover Publications, Inc., 1972.

[4] Y. Chen, C. Zhou, and L. Jing, “Modeling coupled THM processes of geological porous media with multiphase flow: Theory and validation against laboratory and field scale experiments,” *Comput. Geotech.*, vol. 36, no. 8, pp. 1308–1329, Oct. 2009.

[5] T. Zhang, “Modeling of Nanoparticle Transport in Porous Media,” University of Austin Texas, 2012.

[6] C. Wang, A. D. Bobba, R. Attinti, C. Shen, V. Lazouskaya, L.-P. Wang, and Y. Jin, “Retention and transport of silica nanoparticles in saturated porous media: effect of concentration and particle size.,” *Environ. Sci. Technol.*, vol. 46, no. 13, pp. 7151–8, 2012.

[7] M. Tyagi, P. Jenny, I. Lunati, and H. A. Tchelepi, “A Lagrangian, stochastic modeling framework for multi-phase flow in porous media,” *J. Comput. Phys.*, vol. 227, pp. 6696–6714, 2008.

[8] M. Tyagi, “Probability Density Function Approach for Modeling Multi-Phase Flow in Porous Media,” 2010.

[9] D. W. Dean, “An analysis of the stochastic approaches to the problems of flow and transport in porous media,” University of Colorado, 1997.

[10] M. Bargiel and E. M. Tory, “Stochastic dynamic solution of nonlinear differential equations for transport phenomena,” *AIChE J.*, vol. 42, no. 3, pp. 889–891, 1996.

MULTI-SCALE AND MULTI-UNCERTAINTY MODELING OF ENERGY HARVESTERS UNDER ENVIRONMENTAL VIBRATIONS

Claudio Maruccio[1,*], Giuseppe Quaranta[2], Francesco Trentadue[3], Giuseppe C. Marano[4]

[1]Department of Innovation Engineering, University of Salento, via Monteroni, 73100, Lecce, Italy

[2]Department of Structural and Geotechnical Engineering, Sapienza University of Rome, via Eudossiana 18, 00184, Rome, Italy

[3]Department of Civil Engineering and Architecture, Technical University of Bari, via Orabona 4, 70125, Bari, Italy

[4]College of Civil Engineering, Fuzhou University, No. 2 Xue Yuan Road, University Town, 350108, Fuzhou (Fujian), P.R. China.

Localization and homogenization conditions for electro-mechanically coupled problems are recently derived in Ref. 1. Moreover, two scale homogenization procedures were also proposed for electromechanical solids at, both, small deformation (Ref. 2) and finite strains (Ref. 3). However, these approaches are limited to static analysis and, unfortunately, most of electromechanical devices operate under dynamic loading. Extension of the multilevel finite element techniques to dynamic applications leads to a huge computational cost not available in the current practise. At the same time, a lot of research focuses on development of reduced order modeling procedures for MEMS and NEMS applications. These approaches present several advantages: mainly, they allow to include effects of parameter uncertainties in the design and to optimize energy harvester performances (Ref. 4 and Ref. 5).

In this paper, a computational approach for multi-scale and multi-uncertainty modeling of energy harvesting devices under environmental vibration is proposed. Three different levels are considered within a bottom-up approach: micro, macro and system level scales. Transition from micro to macro quantities is based on Hill's energy principle while we show that transfer from macro to system level variables is possible if special conditions are satisfied at the macroscale.

A vibration based energy harvesting device is used to assess the capability of the proposed computational procedure. Stationary and non-stationary base excitations are considered and the uncertainty levels due to intrinsic randomness are assessed in terms of displacement and output voltage responses. At the same time, since the overall state space description is based on lumped coefficients enriched with information derived by the multiscale simulations, micro and macro stress/strain and electric potential distributions are also predicted with a good accuracy.

References

[1] Schroeder J., 2009. Derivation of the localization and homogenization conditions for electro-mechanically coupled problems. Comput. Mater. Sci., 46, (3), pp. 595-599.

[2] Schroeder J., Keip M. A., 2012. Two scale homogenization of electromechanically coupled boundary value problems. Comput. Mech. 50, pp. 229-244.

[3] Keip M. A., Steinmann P., Schroeder J., 2014. Two scale computational homogenization of electro-elasticity at finite strains. Comput. Methods Appl. Mech. Engrg., 278, pp. 62-79.

[4] Nayfeh A. H., Younis M. I., Abdel-Rahman E. M., 2004. Reduced-Order Models for MEMS Applications. Nonlinear Dynamics, Vol. 41, Issue 1, pp. 211-236.

[5] Bechtold T., Schrag G., Feng L., 2013. System-Level Modeling of MEMS. Wiley-VCH Verlag GmbH & Co. KGaA. ISBN: 9783527319039.

THERMO – HYDRO – MECHANICAL MODEL OF MULTIPHASE FLOW IN HYDROCARBON RESERVOIRS WITH NON-EQUILIBRIUM MASS TRANSFER PHENOMENA

López, E.A.[1,*], Mejía, J.M.[2], Chejne, F.[3]

[1]Dinámica de flujo y transporte en medios porosos, ealopez@unal.edu.co

[2]Dinámica de flujo y transporte en medios poroso, jmmejiaca@unal.edu.co

[3]Termodinámica aplicada y energías alternativas, fchejne@unal.edu.co

Multiphase flow in a porous materials, such as hydrocarbon reservoirs, depends on geometrical, petrophysical, operational variables and thermodynamic/transport fluid properties as well. Thermo-Hydro-Mechanical (THM) models emerged in the last 15 years for dealing with these strongly coupled phenomena having a profound impact on the flow behavior, and hydrocarbon production in oil and gas reservoirs. However, recent incremental production strategies such as chemical recovery methods using polymers, surfactants, alkalis and, more recently, nanofluids, involve additional phenomena not accounted for in the THM models. These phenomena includes adsorption, desorption, dissolution, aggregation and other. The problem becomes more complex when these mass transfer phenomena has a dynamic behavior, i.e. components evolve in the multiphase system under non-equilibrium conditions. The general picture of these systems result in multiscale & multiphysics problem [1], [2], [3].

Subsequently, a theoretical treatment for non-isothermal and non-equilibrium transport and deformation phenomena in saturated porous media is presented in this work. The model accounts for multiphase and multicomponent transport in porous media, where temperature, pressure and stresses fields act on the system. The model equations are based on three laws: Mass conservation, energy conservation and mechanical equilibrium, as follows:

- In the mass balance equations, a multicomponent approach is followed. Three compressible phases (oil, brine and gas) are present, where partial miscibility of gas in both water and oil is included [1], [2]. In addition, phases are expressed in terms of components existing in one or more phases. These components can be hydrocarbons, nanoparticles, polymers, surfactants, etc. Components from one phase can be transferred to other phases by any mass transfer mechanism, such as adsorption, dissolution, etc. Mass transfer phenomena can occur under equilibrium or non-equilibrium conditions.
- The geomechanical constituent is a poro-elasto-plastic model, which considers both lineal and non-lineal elastic and plastic behavior of the solid phase (little local deformations are assumed for a given time-step) [4] – [9]. A failure criterion, such as the Cam – Clay or Drucker – Prager criteria [10], is used for yield point identification.
- In the energy transport equation, a local thermal equilibrium between solid and fluid phases is assumed. Energy transport mechanisms include advection and diffusion [8], [9], [11].

Each equation contains terms that accounts for the interaction with other equations, generating a strongly coupled model. In addition, constitutive equations must be specified in order to develop a strategy for the numerical solution [10], [11].

When dynamic transfer mechanism are specified, the numerical solution strategy must face two problems: i). The number of partial differential equation increases; ii). Multiple time-scales are present because different mass transfer time-scales exist and these might be different from the flow time-scale. The paper address a general algorithm for dealing with such a problems.

The contribution of this paper is focused to the description and knowledge of transport in porous media. Specifically, it presents the general form of flow equations, related to flowing phases and components equation, considering mass transport phenomena under non-equilibrium state such as: sorption, dissolution, aggregation, deposition, etc.

References

[1] J. Lee, J. Rollins, and J. Spivey, Pressure Transient Testing, First edition. Richardson,Texas, USA: SPE Textbook Series, 2003

[2] A. U. Chaudhry, Oil well testing handbook, First edition. Houston, Texas: Elsevier Inc., 2004.

[3] T. Zhang, "Modeling of Nanoparticle Transport in Porous Media," University of Austin Texas, 2012.

[4] R. I. Borja, Plasticity Modeling & Computation. First edition. Stanford, Caliornnia. Springer, 2013.

[5] P. A. Charlez, Rock Mechanics: Theoretical Fundamentals, First edition. Paris: Editions Technip, 1991.

[6] J. C. Jaeger, N. G. W. Cook, and R. W. Zimmerman, Fundamentals of rock mechanics, Fourth edition. USA: Blackweell publishing, 2007.

[7] O. Coussy, Mechanics and Physics of Porous Solids, First edition. Chicehter: John Wiley & Sons, 2010.

[8] Y. Chen, C. Zhou, and L. Jing, "Modeling coupled THM processes of geological porous media with multiphase flow: Theory and validation against laboratory and field scale experiments," Comput. Geotech., vol. 36, no. 8, pp. 1308–1329, Oct. 2009.

[9] N. Khalili and B. Loret, "An elasto-plastic model for non-isothermal analysis of flow and deformation in unsaturated porous media : formulation," Int. J. solids Struct., vol. 38, pp. 8305–8330, 2001.

[10] R. Davis and A. P. S. Selvadurai, Plasticity and geomechanics, First edition. Cambridge university press, 2002.

[11] J. Bear and M. Y. Corapcioglu, "A mathematical model for consolidadtion of thermoelastic aquifer due to hot water injection or pumping," Water Resour. Res., vol. 17, pp. 723–736, 1981.

A Practical Comparison Between The Spectral Wiener Chaos Expansions In Solving the Stochastic Differential Equations (SDEs)

Mohamed A. El-Beltagy[1,*], Amnah S. Al-Johani [2]

[1] Cairo University, Engineering Faculty, Egypt, zbeltagy@eng.cu.edu.eg

[2] Tabuk University, Faculty of Science, Saudi Arabia, xxwhitelinnetxx@hotmail.com

In this abstract, we will discuss and compare solving SDEs using the stochastic spectral methods. As in [1], there are, at least, two chaos expansions. The first is the Wiener-Itô expansion (WIE) or it is also known in the literature as Wiener-Hermite expansion (WHE) , [2]. The second expansion is the Wiener Chaos expansion (WCE), suggested in [3].

In WHE, the basis functions are the white noise processes and the solution process is written as an infinite series of iterated Itô integrals. Practically, the expansion is truncated after few $M+1$terms according to the required approximation [4] :

$$u(t;\omega)=\sum_{k=0}^{M}\int_{R^k}u^{(k)}dB_1(t)\cdots dB_k(t)=\sum_{k=0}^{m}\int_{R^k}u^{(k)}H^{(k)}d\tau_k$$

Where $B(t)$ is the Brownian motion, $u^{(k)}(t;t_1,t_2,\cdots,t_k)$ is the k^{th} deterministic kernel of $u(t;\omega)$, $H^{(k)}\left(W(t_1),W(t_2),\cdots,W(t_k)\right)$ is a k^{th}-order symmetric Hermite polynomial in the white-noise porocesses and $\tau_k=t_1t_2\cdots t_k$. The mean and variance are computed as [4]:

$$E[u]=u^{(0)}\quad\text{and}\quad Var[u]=\sum_{k=1}^{M}k!\int_{R^k}\left(u_i^{(k)}\right)^2d\tau_k$$

In WCE, the basis functions are Wick polynomials $T^{(\alpha)}$, each polynomial is the tensor product of Hermite polynomials in K i.i.d random variables $\{\zeta_i\}_{i=1}^{K}$. The solution is expanded as a sum of a product of deterministic kernels $u^{(\alpha)}$ and $T^{(\alpha)}$, i.e.

$$u(t;\omega)=\sum_{\alpha\in J}u^{(\alpha)}T^{(\alpha)}$$

Where J is the set of all multi-index vectors α with K integers such that $|\alpha|\le N$. The mean and variance are computed as [5]:

$$E[u]=u^{(\alpha=0)}\quad\text{and}\quad Var[u]=\sum_{\alpha\neq0}\left(u^{(\alpha)}\right)^2$$

We can notice that WHE basis is a limit of WCE basis with infinite number of random variables included implicitly in the white-noise functions. This is an advantage since WHE is truncated in one dimension only (number of terms $M+1$ in the chaos expansion), while WCE is truncated in two dimensions (the number of random variables K and the highest order N of Wick polynomials).

WHE produces a system of integro-differential equations in the kernels $u^{(k)}$ while WCE produces a regular system of differential equations in the kernels $u^{(\alpha)}$. In both techniques, the resulting deterministic system will be coupled if the SDE is nonlinear and/or the noise term is of multiplicative type. The resulting system using WHE is more complicated and it can be simplified using some techniques e.g. perturbation technique [6].

In both techniques, the equivalent deterministic system is obtained by writing the solution in its chaos expansion and then multiplying by $H^{(k)}; 0 \le k \le M$ in WHE or $T^{(\alpha)}$; $\alpha \in J$ in WCE and take the expectation $\langle \cdots \rangle$. As an example, let us consider the geometrical Brownian motion SDE,

$$L(u) = \frac{du}{dt} - r\,u = \sigma\, u\, W(t) \qquad ; u^{(k=0)}(0) = u^{(\alpha=0)}(0) = u_0$$

Where the white-noise $W(t) = dB(t)/dt$ and L is a linear operator. Applying both techniques as above to get the following equivalent deterministic system.

WHE system: $$L\left(u^{(j)}\right) = \sigma \sum_{k=0}^{M} \int_{R^k} u^{(k)} \left\langle W(t)\, H^{(k)} H^{(j)} \right\rangle d\tau_k \qquad ; \qquad j \le M$$

WCE system: $$L\left(u^{(\alpha)}\right) = \sigma \sum_{\beta \in J} \sum_{i=1}^{\infty} u^{(\beta)} m_i \left\langle \xi_i\, T^{(\alpha)} T^{(\beta)} \right\rangle \qquad ; \qquad \alpha \in J$$

Where m_i ; $i \ge 1$ is a set of orthonormal basis [5]. In both techniques, we can notice that the mean kernel is affected directly by the Gaussian kernel(s) which in turn affected by higher-order non-Gaussian kernels. The resulting deterministic system can be solved using any suitable analytic or numeric scheme, see for example [7].

References

[1] Holden, H., Øksendal, B., Ubøe, J., Zhang, T., 2010. Stochastic Partial Differential Equations A Modeling, White Noise Functional Approach. Springer-Verlag, New York.

[2] Imamura, T., Meecham, W., Siegel, A., 1965. Symbolic Calculus of the Wiener Process and Wiener–Hermite Functionals. Journal of Mathematical Physics, 6, 695-706.

[3] Cameron, R.H., Martin, W.T., 1947. The Orthogonal Development of Non-linear Functionals in Series of Fourier–Hermite Functionals. Annals of Mathematics, 48, 385–392.

[4] El-Beltagy, M.A., El-Tawil, M.A., 2013. Toward a Solution of a Class of Non-Linear Stochastic perturbed PDEs using Automated WHEP Algorithm. Applied Mathematical Modelling, 37, 7174–7192.

[5] Luo, W., 2006, Wiener Chaos Expansion and Numerical Solutions of Stochastic Partial Differential Equations. Ph.D. thesis, California Institute of Technology, Pasadena, California, United States.

[6] El-Beltagy, M.A., Al-Johani, A.S., 2013. Higher-Order WHEP Solutions of Quadratic Nonlinear Stochastic Oscillatory Equation, Engineering, 5, 5A, 57-69.

[7] Lord, G. J., Powell, C. E., Shardlow, T., 2014. An Introduction to Computational Stochastic PDEs. Cambridge University Press, New York.

Multi-Scale Stochastic Damage Model and Its Application to Shearwall Structure

Xiaodan Ren[1,*], Decheng Feng[2], Jie Li[3]

[1]Tongji University, rxdtj@tongji.edu.cn

[2]South East University, dcfeng@seu.edu.cn

[3]Tongji University, lijie@tongji.edu.cn

Concrete is the most used construction materials in the world. When subjected to external loads, cracks propagate within concrete and the structures degrade. The most adopted model for the degradation modelling of concrete is the damage model. On the other hand, concrete is heterogeneous in its nature. Thus the behaviors of concrete is rather different even for the specimens cast from the same batch of concrete. This could be considered as the randomness of concrete. To handle the degradation and randomness of concrete in a unified model, the stochastic damage model is proposed. The micro-cracking of concrete is considered by the rupture of micro-element. The distributive cracking is considered by a random field described by the marginal probability density function and correlation function. The evolution of damage, which represents the degradation of stiffness in the macro-level, is developed based on a filtered random integration over the random field. We have

$$D = \frac{1}{A_\Omega}\int_\Omega H\left[\varepsilon - \Delta(\mathbf{x})\right]dA \tag{1}$$

To determine the stochastic damage evolution in Eq. (1), a random functional method is proposed. The random field $\Delta(\mathbf{x})$ is condensed into two random variables by the random functional method. And the stochastic nonlinear analysis of concrete structures could be easily performed.

Based on the proposed stochastic damage model and implementation scheme, a shear wall is simulated as a numerical example. The stochastic damage evolution of concrete yields random responses of structure. According to the results, we could observe the suppression and exaggeration of randomness between material level and structural level. And the evolution of probability density is a perfect tool to represent the evolution randomness within nonlinear system.

References

[1] Li, J. and Ren, X.D., 2009. Stochastic damage model for concrete based on energy equivalent strain. International Journal of Solids and Structures, 46(11-12), 2407–2419.

[2] Li, J. and Chen, J.B., 2009. Stochastic Dynamics of Structures. John Wiley & Sons.

Uncertainty Analytics in a Computational Model

Heonjun Yoon[1], Byeng D. Youn[1]*, Heungsoo Kim[2], Chang-Kyung Ryoo[3]

[1]Department of Mechanical and Aerospace Engineering, Seoul National University, Seoul 08826, Republic of Korea

[2]Department of Mechanical, Robotics, and Energy Engineering, Seoul 100-715, Republic of Korea

[3]Department of Aerospace Engineering, Incheon 22212, Republic of Korea

* Corresponding author (Tel: +82-2-880-1919; E-mail: bdyoun@snu.ac.kr)

Virtual testing has been widely recognized as of great importance in designing and evaluating an engineered product. In many engineering problems, the construction of a computational model for virtual testing starts by deriving an ordinary differential equation (ODE) governing the physics of interest. Since there inherently exist uncertainty and complexity in reality, the ODE-based computational models in a deterministic form fail to emulate accurately the behaviors of the engineered product. The uncertainty effects thus have to be taken into account to improve the predictive capability of the ODE-based computational model, indicating the necessity of 'engineering analysis and design under uncertainty'. Despite advances in uncertainty quantification and propagation methods, however, there is still a great need for a systematic framework that elucidates (1) how to consolidate the effects of different kinds of uncertainty in the input quantities on the output responses, (2) how to incorporate uncertainty arising from conscious approximations in modeling, lack of data, and being incognizant of incomplete knowledge. The primary objective of this study is thus to make steps forward to a comprehensive understanding of the uncertainty effects on the predictive capability of the ODE-based computational model in accordance with uncertainty analytics. This uncertainty analytics provides taxonomy to classify and identify the source and type of uncertainty in engineering analysis and design. The source is divided into 'physical', 'model form', and 'statistical' uncertainty, while the type includes 'aleatory' and 'epistemic' uncertainty. Depending on the awareness of the existence, epistemic uncertainty is further divided into 'recognized' and 'unrecognized blind' uncertainty. The contribution of this study lies in that we provide an insightful guideline on how to manage uncertainty in the decision-making process for developing the engineered product in a cost-effective manner.

POSTBUCKLING OF GRAPHENE SHEETS

Nuno Silvestre[1,*], Bruno Faria[2], José N. Canongia Lopes[2], Cátia Guarda[1]

[1] IDMEC, Department of Mechanical Engineering, Instituto Superior Técnico, University of Lisbon, Av. Rovisco Pais, 1049-001 Lisboa, Portugal, nsilvestre@ist.utl.pt

[2] CQE, Department of Chemical and Biological Engineering, Instituto Superior Técnico, University of Lisbon, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

This paper focuses on the postbuckling behaviour of single layer graphene sheets (SLGS) at nanoscale. In order to study this topic, molecular dynamics (MD) models of graphene sheets were developed. The shhets have rectangular shape with dimensions (L=300 Å, W=150 Å), aspect ratio L/W=2, ~18000 carbon (C) atoms, armchair and zigzag configurations, and have all edges simply supported. The LAMMPS software was used, the AIREBO potential was adopted for C-C bonds, Lennard-Jones 12-6 potential was used for non bonded C atoms, the Nosé-Hoover thermostat at 300 K temperature was considered and the NVT ensemble was adopted. Regarding the loading procedure and MD simulations, an initial equilibration was considered (MD with TS=0.5 fs + 10.000 TS to stabilize SLGS, each structural analysis comprises 2.000 MD simulations (increments), the increment is a displacement of 0.1 Å imposed at both (top + bottom) boundaries of SLGS (ΔL= - 0.2 Å / increment), the MD simulation has 10.000 TS, each TS= 1 fs, and the strain energy was recorded and averaged for the last 3.000 TS. The MD results comprised the variation of energy with the compressive strain, the variation of compressive force with the imposed displacement, and the failure modes. Figures 1 and 2 show the force-displacement curves and failure modes of SLGS with similar aspect ratio (L/W=2) but different chirality (armchair vs. zigzag).

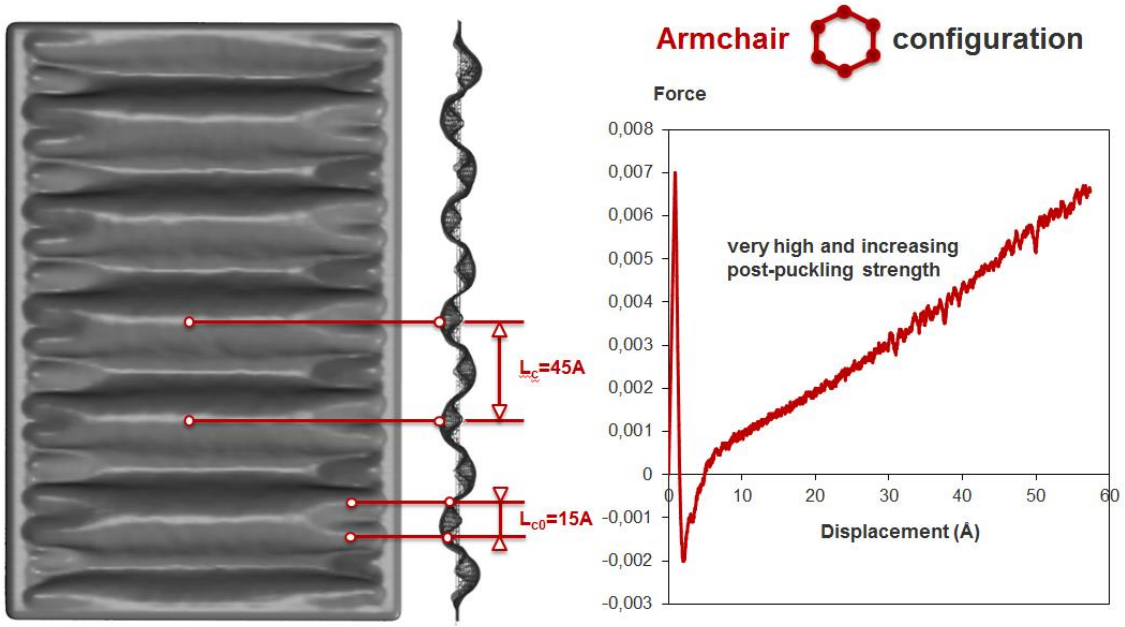


Figure 1. Force-displacement curve and failure mode of armchair SLGS with aspect ratio L/W=2

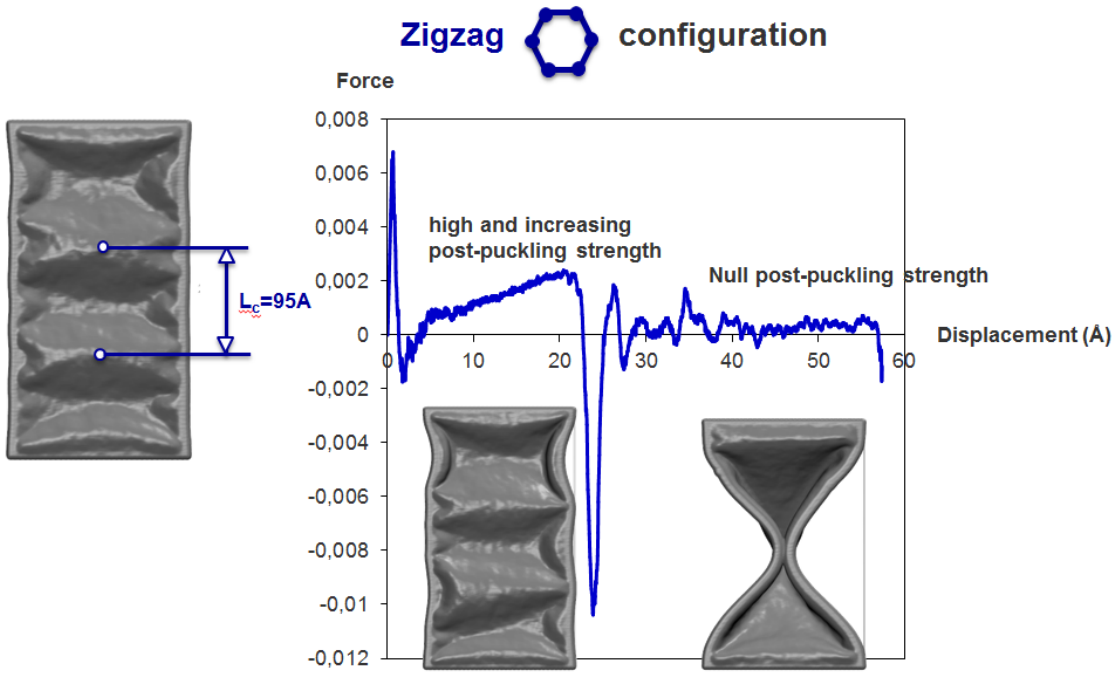


Figure 2. Force-displacement curve and failure mode of zigzag SLGS with aspect ratio L/W=2

The results show that the critical buckling load is approximately the same for both cases (armchair and zigzag) but the buckling mode shape is markedly different: the armchair SLGS buckles in 11 halfwaves with very short wavelength while the zigazag SLGS buckles in 5 halwaves with moderate wavelength. The initial postbuckling behaviour is also similar for both SLGS, being stable because the load increases with the increasing displacement. However, for compressive strains beyond 7% the different mode shape has a severe impact on the postbuckling behaviour: the armchair SLGS keeps its stable behaviour (positive slope of force-displacement curve) while the zigzag SLGS shows a secondary bifurcation and the mode jumps into another mode with a single halfwave, which has no postbuckling stiffness and strength. A limited study was also performed to investigate the effect of aspect ratio on the postbuckling behaviour of SLGS. It was shown that increasing the aspect ratio L/W leads to an unexpected increase of the critical buckling load but also to a decrease of the postbuckling strength of the SLGS, regardless the SLGS chirality.

References

[1] Silvestre, N., 2015. Non-Linearity and Anisotropy at Nanoscale. Plenary Lecture, 18th International Conference on Composite Structures (ICCS18), Lisbon, Portugal, June 15-18, 2015.

FULLY SCALABLE IMPLEMENTATION OF A VOLUME COUPLING SCHEME FOR THE MODELING OF RANDOM POLYCRYSTALLINE MATERIALS

R. Cottereau[1], T. Milanetto Schlittler[1]

[1] Laboratoire MSSMat, CNRS, CentraleSupélec, Université Paris-Saclay, France

regis.cottereau@centralesupelec.fr

Abstract

This contribution presents a new implementation of a multi-scale, multi-model stochastic-deterministic coupling algorithm, with a proposed parallelization scheme for the construction of the coupling terms between the models. This allows one to study such problems with a fully scalable algorithm on large computer clusters, even when the models and/or the coupling have a high number of degrees of freedom. As an application example, we will consider a system composed by a homogeneous, macroscopic elasto-plastic model and a stochastic heterogeneous polycrystalline material model, with a volume coupling based on the Arlequin framework.

Introduction

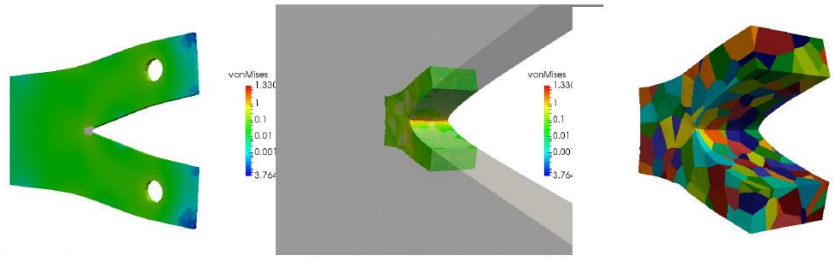
Coupling methods, in general, allow the study of multi-scale systems, taking into account the different physical processes at each scale. These methods can be classified in several different types, depending on the desired application. Methods like the VMS [1] and the HMM [2], and similar others, are used when themacro-scale's model parameters are not known, but depend on the micro-scale over the whole domain. They can be classified as embedding methods, with the VMS enriching the macro-scale with the micro-scale model over element patches, and the HMM altering the quadrature evaluation of the weak formulation. If, on the other hand, the macro-scale quantity of interest depends on the micro-scale only over a part of the former's domain, more local methods are used. Examples include the non-overlapping domain decomposition methods. They are derived from domain decomposition techniques developed to solve numerically PDEs over large-scale computer clusters [3], and they are used when the coupling is done overan interface between the models.

For overlapping domains, still in the context of a limited domain coupling, methods based on volume couplings can be used, such as the Arlequin framework [4,5,6] and the bridging domain method [7]. They keep the same weak formulation as the other methods but differ from the interface methods by defining a volume coupling over the overlapping domains. These methods differ mainly on the choice of this coupling term. In both cases, the coupling matrix is built using an intermediary mesh, constructed by meshing the geometrical intersections between the elements of the macro and micro domain meshes. Finally, methods such as Nitsche method [8] have points in common with both the interface and volume couplings. There is a volume overlap between the models, but the formulation defines the coupling over an interface between the overlapping domains only.

Generally speaking, the coupling step is not parallelized for methods following the formulations above. In many cases, this is justified because the mediator space is smaller when compared to the models associated with it. However, as a consequence, even when the parallel implementations associated to each of the numerical models scale well, the serial coupling step breaks this scalability of the algorithm as a whole. Previous works using the coupling algorithms and parallelism focused on simulating several couplings

between a single global model and many local models, with each coupling being associated to one processor [6]. Here, we use a different approach, and present a version of the Arlequin

framework with a parallelized and scalable coupling step. The consideration of the coupling of deterministic and stochastic models is done in [9,10].. As an example of this implementation, we study a coupled system formed by a macroscopic and homogeneous elasto-plastic model and a polycrystalline material model (see illustration below). While we focus on this example here, this framework – and thus this implementation – can be applied to other cases involving multi-scale physics, such as the ones cited above. Similarly, we insist that, while we focus here in the Arlequin framework, the parallelization scheme presented here is applicable to any coupling methods using similar formulations.



Example of macro-micro coupled model

Zoom on micro-scale model

Zoom on micro-scale deformations

This work benefited from French state funding managed by the National Research Agency under project number ANR-14-CE07-0007 CouESt.

References

[1] Hughes, T.J.R.: Multiscale phenomena: Green's functions, the Dirichlet-to-Neumann formulation, subgrid scale models, bubbles and the origins of stabilized methods. Computer Methods in Applied Mechanics and Engineering 127(1–4), 387–401 (1995). DOI 10.1016/0045-7825(95)00844- 9

[2] E, W., Engquist, B.: The Heterogeneous Multiscale Methods. Communications in Mathematical Sciences 1(1), 87–132 (2003). DOI 10.4310/CMS.2003.v1.n1. A8

[3] Dolean, V., Jolivet, P., Nataf, F.: An Introduction to Domain Decomposition Methods. Society for Industrial and Applied Mathematics (2015)

[4] Dhia, H.B.: Problèmes mécaniques multi-échelles: la méthode Arlequin. Comptes Rendus de l'Académie des Sciences – Series IIB – Mechanics- Physics-Astronomy 326(12), 899–904 (1998). DOI 10.1016/S1251-8069(99)80046- 5.

[5] Néron, D., Dhia, H.B., Cottereau, R.: A decoupled strategy to solve reduced-order multimodel problems in the PGD and Arlequin frameworks. Computational Mechanics pp. 1–13 (2016). DOI 10.1007/s00466- 015-1236- 0

[6] Dhia, H.B., Elkhodja, N., Roux, F.X.: Multimodeling of multi-alterated structures in the Arlequin framework.European Journal of Computational Mechanics 17(5-7), 969–980 (2008). DOI 10.3166/remn.17. 969- 980.

[7] Xiao, S., Belytschko, T.: A bridging domain method for coupling continua with molecular dynamics.Computer Methods in Applied Mechanics and Engineering 193(17- 20), 1645–1669 (2004). DOI 10.1016/j.cma.2003.12.053.

[8] Massing, A., Larson, M.G., Logg, A.: Efficient implementation of finite element methods on non-matching and overlapping meshes in 3D. arXiv:1210.7076 [math] (2012).

[9] Cottereau R., Clouteau D., Ben Dhia H., Zaccardi C.. A stochastic - deterministic coupling method for continuum mechanics. Computer Methods in Applied Mechanics and Engineering, 200(47-48), 3280-3288,(2011).

[10] Le Guennec Y., Cottereau R., Clouteau D., Soize C.. A coupling method for stochastic continuum models at different scales. Probabilistic Engineering Mechanics, 37, 138-147, (2014).

SUPPLY CHAIN EQUILIBRIUM UNDER TWO TYPES OF UNCERTAINTY: CASTOMERS DEMAND AND SUPPLIERS LEADTIME

Konstantin Kogan[1,*], Tal Avinadav[2], Tatyana Chernonog[3]

[1]Department of Management, Bar-Ilan University, Israel, kogank@biu.ac.il

[2] Department of Management, Bar-Ilan University, Israel, Tal.Avinadav@biu.ac.il

[3] Department of Management, Bar-Ilan University, Israel, Tatyana.Chernonog@biu.ac.il

Much research has been conducted to handle two major sources of uncertainty that the retail industry faces—customers' demand and suppliers' leadtime (see, e.g., Zou et al. [1], Dolgui et al. [2]). These uncertainties result either in stock-outs or over-stocks, and cause massive losses to the retailers every year. We consider the effect of competition between a firm (retailer) and its supplier on their decisions. The supply chain parties interact via a wholesale price contract with risk sharing via penalties paid by the supplier to the firm for early/late supplies. Both the demand for products and the delivery leadtime are stochastic. We use Nash and Stackelberg scenarios to model the competition with a game theoretic approach depending on the level of information available to the supply chain parties. The Stackelberg scenario assumes the supplier is the leader. This power balance reflects a supplier who is aware of the retailer's operational data, and therefore is able to assess the retailer's behavior, but not vice versa. The Nash scenario implies the supply chain parties are fully transparent. In both approaches the firm determines the order quantity and the planned delivery time, whereas the supplier controls the accuracy of the deliveries.

We find that supplier's leadership has no effect on the supply chain equilibrium only if the system conditions are such that the demand is known and an order should be placed as soon as possible. Further, our computational experiments unexpectedly show, the Stackelberg solution, and therefore information assymetry, may be more profitable for both supply chain parties, i.e., it is pareto-improving. We also find that by agreeing to greater compensations for early and late deliveries, the supplier may increase its expected profit as well as the profit of the entire supply chain, thereby coordinating it.

References

[1] Zou, X., Pokharel, S., Piplani, R., 2004. Channel coordination in an assembly system facing uncertain demand with synchronized processing time and delivery quantity. *International journal of production research 42*(22), 4673-4689.

[2] Dolgui, A., Ammar, O. B., Hnaien, F., Louly, M. A. , 2013. A state of the art on supply planning and inventory control under lead time uncertainty. Studies in Informatics and Control 22(3), 255-268.Geers, M., 1997. Experimental Analysis and Computational Modelling of Damage and Fracture. Ph.D. thesis, Eindhoven University Of Technology, Eindhoven, The Netherlands.

Comparison between stochastic and possibilistic evaluation of rubber materials

Ismail Caylak[1,*], Alex Dridger[2], Eduard Penner[3], Rolf Mahnken[4]

[1]Chair of Engineering Mechanics (University of Paderborn), caylak@ltm.upb.de

[2]Chair of Engineering Mechanics (University of Paderborn), dridger@ltm.upb.de

[3]Chair of Engineering Mechanics (University of Paderborn), penner@ltm.upb.de

[4]Chair of Engineering Mechanics (University of Paderborn), mahnken@ltm.upb.de

Components and structures, e.g. made of adhesives, polycristallines and composites, are heterogeneous. This heterogeneity leads to uncertainties in the system response, whereby various causes can be responsible for this. In this work, we restrict ourselves to uncertainties due to fluctuating material parameters. When assessing the reliability of components and structures, uncertainties are distinguished into aleatoric and epistemic uncertainty [1]. The aleatoric uncertainty can be regarded as a stochastic uncertainty. This means that the statistics are known for stochastic quantities. Epistemic uncertainties, on the other hand, arises due to a lack of knowledge, i.e. due to incomplete and/or imprecise information. The aim of this contribution is to compare both kinds of uncertainty. For the aleatoric uncertainty, the mechanical system must be described by stochastic partial differential equations (SPDEs). The solution of the mathematical problem can be done numerically using the stochastic finite element method (SFEM). A widely used numerical simulation method for solving SFEM is the Monte Carlo method [2,3] which results into significant computational effort. An alternative method to reduce the computational effort, is the spectral stochastic finite element method (SSFEM), which was proposed by Ghanem and Spanos [4] and presented in a comprehensive monograph by Ghanem and Spanos [5]. This method is based on polynomial chaos expansions (PCE), which allows one to represent a random variable as Fourier series of orthogonal polynomials. For elastomers, we refer to [6] where the SSFEM for large deformation problems is proposed.

The epistemic uncertainty requires a non-stochastical approach. Interval FEM and fuzzy FEM (FFEM) [7] are methods to comprise the epistemic uncertainty in the simulation. In the interval FEM the uncertainties in the design variables are expressed by interval values and the interval arithmetic technique is used to solve the equation system in the interval FEM. The design variables in the FFEM are characterized by fuzzy sets and membership functions, respectively, which were introduced to represent data and information possessing non-statistical uncertainties.

The ensemble of both types of uncertainty is referred to as imprecise probability and is able to deal with sparse experimental informations. Zadeh [8] introduced the possibility theory based on the fuzzy set theory which was further developed by Dubois and Prade [9] in order to deal with imprecise probabilities. According to [9] the possibility theory constitutes the simplest uncertainty theory devoted to the modeling of incomplete information, and thus, forms a suitable approach in order to deal with sparse experimental information for design variables such as material parameters in the (fuzzy) finite element method.

Our work describes the stochastic and possibilistic evaluation of the stochastic and fuzzy modeling of Ogden's material model at large deformations. The statistics for stochastic

evaluation are given from experiments of rubber materials. For possibilistic evaluation only sparse experiments are available. The stochastic modeling is based on PC expansion, which requires statistics of material parameters. In the possibilistic approach, material parameters are interpreted as possibility distributions where one of them encodes a family of probability distributions which may occur considering the sparse information of the experimental data. To this end, the probability-possibility transformation is applied to get the required possibility distributions of material parameters. Furthermore, in this work the dependencies between material parameters for both methods will be considered. A comparison with real experimental data will show to what extent both methods agree with reality.

References

[1] Sullivan, T., 2015. Introduction to Uncertainty Quantification. Springer.
[2] Caflisch, R. E., 1998. Monte carlo and quasi-monte carlo methods. Acta numerica 7, 1–49.
[3] Hurtado, J. , Barbat, A., 1998. Monte carlo techniques in computational stochastic mechanics. Archives of Computational Methods in Engineering 5, 3–29.
[4] Ghanem, R. G., Spanos, P. D., 1991. Polynomial chaos in stochastic finite elements. J. Appl. Mech. 57, 197–202.
[5] Ghanem, R. G., Spanos, P. D., 2003. Stochastic finite elements: a spectral approach, Courier Corporation.
[6] Acharjee, S., Zabaras, N., 2006. Uncertainty propagation in finite deformations - A spectral stochastic Lagrangian approach. Computer methods in applied mechanics and engineering 195, 2289–2312.
[7] Moeller, B., and Beer, M., 2004. Fuzzy randomness: uncertainty in civil engineering and computational mechanics. Springer.
[8] Zadeh, L. A., 2006. “Fuzzy sets as a basis for a theory of possibility”. Fuzzy Sets and Systems(1).
[9] Dubois, D., and Prade, H., 2012. Fundamentals of fuzzy sets, Vol. 7. Springer Science & Business Media.

SEMI-INTRUSIVE UNCERTAINTY QUANTIFICATION METHOD FOR MULTISCALE MODELS

Anna Nikishova[1,*], Alfons Hoekstra[2]

[1]Computational Science Lab, University of Amsterdam, A.Nikishova@uva.nl

[2]Computational Science Lab, University of Amsterdam, A.G.Hoekstra@uva.nl

Computer modeling is widely used in science and engineering to study systems of interest and to predict their behaviour. These systems are usually multiscale in nature, as their accuracy and reliability depend on the correct representation of processes taking place on several length and time scales [1]. Such multiscale complex systems are inherently stochastic. Moreover, measurements for model parameters, model validation, or initial and boundary conditions can never be made with perfect accuracy, thus, such data inevitably contain uncertainties [2].

In Uncertainty Quantification (UQ), we distinguish between intrusive and nonintrusive methods to estimate uncertainty in model results [3]. Intrusive methods are efficient and relatively easy to apply to linear model [4]. This, however, represents only a relative small class of models. They can be applied to non-linear models as well, but solution of the resulting equations may become very demanding. Nonintrusive methods can be applied to any type of non-linear models. However, these methods usually require a very large number of model runs [5], which may prohibit using such nonintrusive methods.

We propose an efficient semi-intrusive UQ method for multiscale models with well separated temporal scales, where we reduce the number of samples for the computationally intensive part of multiscale models, i.e. micro scale sub-model (the fast dynamics). In contrast to [6] and [7], in the presented semi-intrusive approach there is no need to perform any modification of the sub-model solvers, but we use the information about the multiscale model structure (Figure 1).

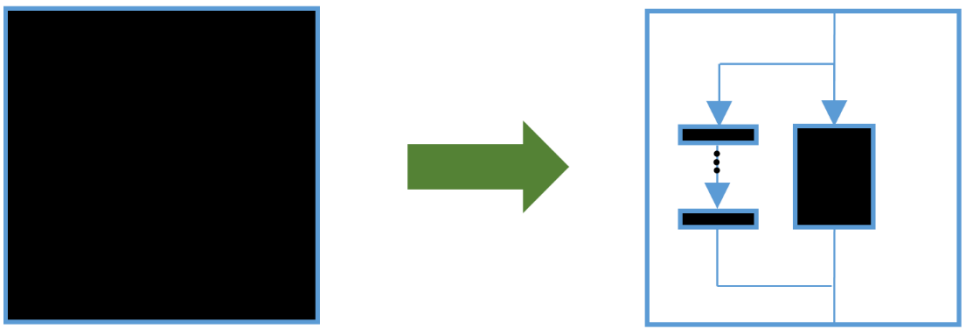


Figure 1. From Black box to Semi-Intrusive Uncertainty Quantification by applying the knowledge about the multiscale model structure

We demonstrate our strategy with a nonintrusive quasi-Monte Carlo method and an intrusive Galerkin method on two case studies based on Reaction-Diffusion dynamics

with random inputs: an one dimensional system with fast diffusion and slow reaction, and a multiscale Grey-Scott model.

We conclude that our approach allows to decrease sufficiently the computational time of UQ in the case of uncertain response for a relatively low-dimensional model as in the first case study. The response of the Grey-Scott model is highly irregular with respect to the uncertain inputs. Moreover, that case study was done in a two-dimensional space. Yet, we still achieved a significant decrease in computational time together with a maximum error in variance about 12% as compared to the UQ using nonintrusive quasi-Monte Carlo.

References

[1] E. Weinan, Principles of Multiscale Modeling, Cambridge University Press, 2011. URL http://www.ebook.de/de/product/14876873/weinan_e_principles_of_multiscale_modeling.html
[2] B. Stephanie, A beginner's guide to uncertainty of measurement (2001).
[3] O. P. L. Maître, O. M. Knio, Spectral Methods for Uncertainty Quantification, Springer Netherlands, 2010. doi:10.1007/978-90-481-3520-2.
[4] X. Wan, G. E. Karniadakis, An adaptive multi-element generalized polynomial chaos method for stochastic differential equations, Journal of Computational Physics 209 (2) (2005) 617–642. doi:10.1016/j.jcp.2005.03.023.
[5] Galitzine, Cyril, and Iain D. Boyd. "An analysis of the convergence of the direct simulation Monte Carlo method." Journal of Computational Physics 289 (2015): 196-223.
[6] A. Mittal, X. Chen, C. H. Tong, G. Iaccarino, A flexible uncertainty propagation framework for general multiphysics systems, SIAM/ASA Journal on Uncertainty Quantification 4 (1) (2016) 218–243. doi:10.1137/140981411.
[7] R. Abgrall, P. M. Congedo, A semi-intrusive deterministic approach to uncertainty quantification in non-linear fluid flow problems, Journal of Computational Physics 235 (2013) 828–845. doi:10.1016/j.jcp.2012.07.041

NUMERICAL STUDY ON THE UNCERTAINTY OF FAILURE PROBABILITY CALCULATION FOR NUCLEAR GRAPHITE COMPONENTS

Hongjie Wang, Xiaoxin Wang, Li Shi*, Haitao Wang, Libin Sun, Xinxin Wu

Institute of Nuclear and New Energy Technology (INET)

Tsinghua University, Beijing, P. R. China

Graphite components are commonly used as reflectors as well as core supporting structure in high temp gas-cooled reactor and are of great importance to the safety of the reactors. As a quasi-brittle material, nuclear graphite shows a large scatter in strength. The probabilistic approach based on weakest link is therefore well suited to evaluate the safety of the graphite components and has been employed in design of graphite internals in HTR. The calculated probabilities of failure (POF), however, are affected by many factors, including the procedure of the calculation, material properties for both unirradiated and irradiated graphite, and methods to analysis the stress in graphite components under reactor environment. To investigate the influences of these factors, a numerical model which is able to consider the material properties change of graphite under irradiation was developed to analysis the stresses of graphite components in the reactor. The POF using different group criterions were calculated and the uncertainties of material properties due to the measurement of the irradiated sample were investigated. The results indicated that the POF was highly sensitive to the group criterions. The grouping method based on grain size is over conservative for fine-grain graphite compared with that based on size of fracture processing zone (FPZ). POF calculated using the strength distribution of unirradiated graphite is generally higher than that using irradiated graphite as the strength of irradiated graphite is increased significantly.

ANALYSIS AND OPTIMIZATION OF HYBRID POLYMER COMPOSITES IN UNIAXIAL TRACTION: ANALITYCAL AND COMPUTATIONAL STUDY

Conde F.M.[1,4,*], Coelho P.G.[2], Tavares R.P.[3], Camanho P.P.[3], Guedes J.M.[4], Rodrigues H.C.[4]

[1] DEMI, Universidade Nova de Lisboa, FCT, 2829-516 Caparica, Portugal, f.conde@campus.fct.unl.pt

[2] UNIDEMI, Faculdade de Ciências e Tecnologia, 2829-516 Caparica, Portugal, pgc@fct.unl.pt

[3] INEGI, Rua Dr. Roberto Frias, 400, 4200-465 Porto, Portugal, {rptavares@inegi.up.pt, pcamanho@fe.up.pt}

[4] IDMEC, Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal, {jmguedes@tecnico.ulisboa.pt, hcr@tecnico.ulisboa.pt}

ABSTRACT

Composite materials have met increasingly interest in industry specially in lightweight construction (for example, in automotive and aerospace applications) due to their special properties compared to the conventional structural materials [1,2]. However, they are characterized by having a brittle failure, i.e. typically they have no ductility, which possibly may limit their usage. A ductile failure of a composite material is desired, like in the metallic materials, which present yielding after the elastic region followed by an increasing of the strength. Hybridization is a key factor to introduce a designated pseudo-ductile behavior [3] in the fiber reinforced composite material. The hybridization here consists in the use of two different types of fibers (with different failure strains or strengths) embedded in a polymer matrix with the goal of improving overall composite properties and performance. The present work analyzes and optimizes this hybrid fiber reinforced composite based on failure analytical models. Ultimately one discovers the optimal mix of fiber materials which produces a ductile behavior in the composite material when it is subjected to a tensile load.

To predict the failure of the composite materials, two different analitycal models developed by Tavares et al. [4,5] are used in this work, which are coupled with optimization algorithms. The first model considers a bundle composed of two different fiber types, without matrix, named by hybrid tows. To account for the presence of the matrix, a second analytical model is used here, based on the multiple fragmentation of the fibers. Despite the simplicity of these failure models, they are very useful to work on a correct parameterization of the response curve of the hybrid composite subject to uniaxial traction. A parameterization of that response is strictly necessary for its control and consequent optimization to achieve the desired pseudo-ductile response. One proposes here four parameters which fully characterize the response. These parameters are included in optimization problems formulated here either using a multi-objective function or a weighted sum of objective functions. The final goal is discovering the optimal mix of the base constituents of the hybrid composite.

As regards the nature of problem design variables, two different types of optimizations are performed here using the aforementioned analytical failure models. Firstly, one formulates and solves a discrete optimization problem and then a continuous one. In the discrete problem the objective is to find, from a database of 20

pre-defined fibers available in the market, the optimal match of fibers for hybridization achieving outstanding pseudo-ductile behavior. In the continuous problem, the objective is discovering the properties of the fibers that could be considered ideal to produce the greatest pseudo-ductile behavior. These two types of optimizations are performed here using typically the Genetic Algorithm (GA) as the optimizer.

Acknowledgements

This work was partially supported by the Portuguese Foundation for Science and Technology, FCT-Portugal, through the projects UID/EMS/00667/2013, UID/EMS/50022/2013 and PTDC/EMS-PRO/4732/2014.

References

[1] Jones, R.M., 1975. Mechanics of composite materials. McGraw-hill.
[2] Mallick, P.K., 1997. Composites Engineering Handbook. Marcel Dekker, Inc.
[3] Yu, H., Longana, M.L., Jalalvand, M., Wisnom, M.R., Potter, K.D., 2015. Pseudo-ductility in intermingled carbon/glass hybrid composites with highly aligned discontinuous fibres. Composites: Part A 73: 35-44.
[4] Tavares, R.P., 2015. Mechanics of hybrid polymer composites. Master's Thesis, University of Porto, Portugal.
[5] Tavares, R.P, Melro, A.R, Bessa, M.A., Turon, A., Wing, K.L., Camanho, P.P., 2016. Mechanics of hybrid polymer composites: analytical and computational study. Comput Mech 57: 405-421.

STATISTICAL HOMOGENIZATION OF A FIBRE NETWORK

Jouni Freund[1*], Alp Karakoç[2]

[1]Aalto University, School of Engineering, Mechanical Engineering, jouni.freund@aalto.fi

[2]University of California Los Angeles, Civil and Environmental Engineering, alpkarakoc@gmail.com

According to experiments, mechanical properties of natural materials like engineered wood require a statistical description to be realistic. In conventional simulations on a deterministic model, the statistical distributions are replaced by measures like mean values or characteristic values. Although computation along these lines is straightforward, reduction in information may lead to a large modelling error. In a non-deterministic simulation, reduction of the data may not be needed. A Monte Carlo type simulation uses a sample of problems to be solved, e.g., by the finite element method. Therefore, a statistical simulation means just a set of deterministic simulations. One of the issues is the scale dependency of the material property statistics which needs to be somehow accounted for in the numerical method used.

The practical way to include the effect of scale in finite element simulations uses the material property statistics as the function of scale. Although finding the representation experimentally is too expensive, use of computational homogenization is possible. A simplistic model for a fiber network, suitable for additive manufacturing and direct testing, is used as an application example. The planar material consists of elastic bands crossing in right angles. First, computational homogenization on a micromechanical model is used to derive the rigidity statistics as function of scale defined by the size of the RVE (Representative Volume Element). After that, equations of plane stress elasticity and the finite element method are used to predict behavior on a scale and geometry where the direct use of a micro-mechanical model is not possible.

References

[1] Stefanou, G., 2009. The stochastic finite element method: Past, present and future. Comput. Methods Appl. Mech. Engrg. 198, 1031–1051.

THERMO-MECHANICAL MODELING OF COMPRESSOR ROOTS: MULTI-PHYSICAL PROBLEMS

Nesrine Hmida[1] , Brahim Tlili [2]

[1] PhD Student at the National School of Engineers of Tunis

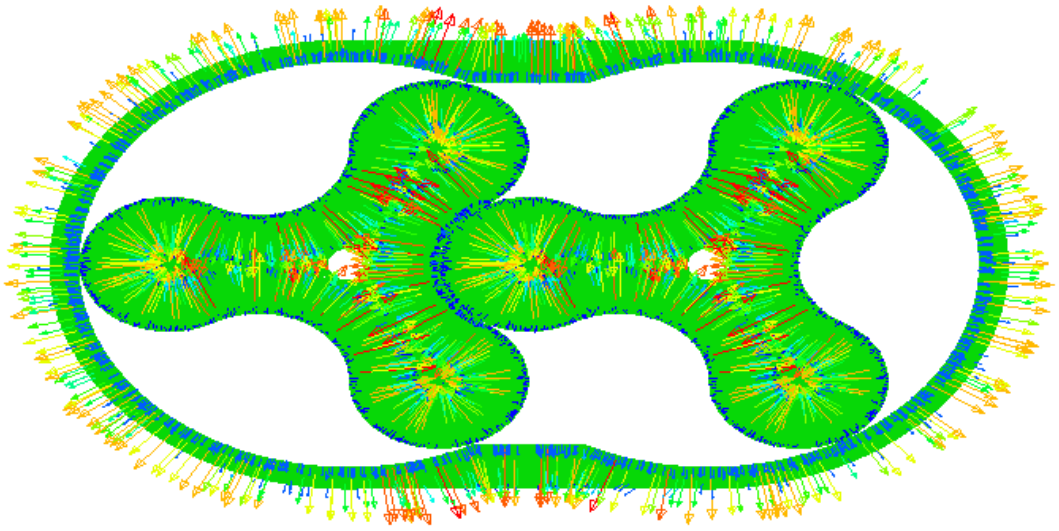
[2] Assistant Professor at the Preparatory Institute for Engineering Studies El Manar

In the case of volumetric compressors, and specially the compressor Roots tri-lobes, the thermo-mechanical modeling highlights several physical phenomena and multi-scale problems. tri-lobe Roots compressor, we opted for a numerical modeling but for which physical parameters are integrated analytically. In this study after having refine the mesh especially in the contact areas, we observed that the criterion of von taken after a full rotor turn reaches the value 1168 Mpa. The two indispensable variables are temperature and thermal flow. The two studied phenomena are conduction (surface to surface) and convection (surface to fluid).

For these reasons several parameters are highlighted, such as temperature, heat flux, the nature of the materials, the rotational speed of the rotors, etc., to solve this type of mechanical and physical problem.

The objective of this work is to provide a model for a better understanding of the thermo-mechanical phenomena responsible for any premature system damage and validate the thermal system. In the thermal system the heat flow is increased, the temperature increases until it stabilizes at 106.7 ° C inside stator after n iterations and 100°C outside stator. The majority of the amount of heat flow on the complete thermo mechanical model is removed from the stator side.

Key words: Compressor, FEA, simulation, thermo- mechanical



ANALYSIS OF PLASTICITY AND WEAR ON A SPHERE-TO-FLAT FRICTIONAL CONTACT

T. Doca[1,*], M.S.T. Pires[1] , V. F. Steier[1], R. Carvalho[2], F. M. A. Pires[2]

[1]University of Brasília, * doca@unb.br

[2] University of Porto

This work employs a sphere-to-flat contact configuration for the analysis of elasto-plastic strains and abrasive wear. The behaviours of the maximum contact pressure and the wear depth are presented as well as the comparison between numerical predictions and measured specimen profiles. For the numerical analysis, the enforcement of the contact constraints is performed using a mortar frictional contact formulation coupled with appropriate finite element technology for the evaluation of large inelastic strains. Moreover, a model for yield surfaces capable to provide correct values of stresses under both traction and shear is employed within the setting of plasticity for a cyclic loading condition. The experimental data is obtained from abrasive wear tests. The main objective is to access the influence of the constitutive model on the evaluation of the wear phenomena. The analysis of results is performed for six different loading configurations and includes all stages of deformation ranging from elastic contact through elasto-plastic deformation to finite deformation plastic contact. The results shown that a better evaluation of the shear stresses leads to a significant improvement of the wear depth prediction.

Keywords: Contitutive modeling, Plasticity, Wear, Frictional contact.

Numerical strategies for a mechanical model based on mixed aleatory and epistemic uncertainties

Amelie Fau[1,*], Mona Dannert[1], Matteo Broggi[2], Udo Nackenhorst[1], Michael Beer[2]

[1]Institut für Baumechanik und Numerische Mechanik, Leibniz Universität Hannover

[2]Institut für Risiko und Zuverlässigkeit, Leibniz Universität Hannover

Most numerical models for engineering applications include uncertainties caused for example, from load, geometry or material properties. Two types of uncertainties may be distinguished, aleatory uncertainties due to random phenomena and epistemic uncertainties due to a lack of knowledge or data [1]. Input variables have generally both, aleatory and epistemic uncertainties. Probability bounds analysis may be used to model such mixed uncertain variables. The probability of an event is here not described by a unique function [2] but within an upper and a lower bound, which form a probability-box (p-box) distribution function. Such models require huge numerical effort [3]. Therefore, collocation and projection methods may be proposed to improve numerical efficiency.

In this work, a stochastic finite element analysis for an elasto-plastic problem involving uncertain constitutive parameters is implemented. The underlying random field is modelled by a p-box. Amongst possible numerical approaches [4], nested collocation scheme, where samples are chosen within a certain lattice construction is examined [5]. The algorithm is tested with one- and two-dimensional examples and verified by Monte Carlo simulation.

References

[1] A. Der Kiureghian and O. Ditlevsen. ``Aleatory or epistemic? Does it matter?" Structural Safety, 31(2), pp. 105-112, 2009.

[2] S. Ferson and J. Hajagos.``Arithmetic with uncertain numbers: rigorous and (often) best possible answers", Reliability Engineering and System Safety, 85(1-3), pp. 135-152, 2004.

[3] H. Zhang et al. Structural reliability analysis on the basis of small samples: An interval quasi-Monte Carlo method, Mechanical Systems and Signal Processing, 37(1-2), pp. 137-151, 2013.

[4] O.P. Le Maitre and O.M. Knio. Spectral Methods for Uncertainty Quantification, Chap. Non-intrusive Methods. Springer, 2010.

[5] D. Xiu and J. S. Hesthaven. High-Order Collocation Methods for Differential Equations with Random Inputs. SIAM J. Sci. Comput., 27(3), pp. 1118-1139, 2005.

PROBABILISTIC METHODS FOR QUANTIFICATION OF UNCERTAINTIES IN PROPERTIES OF HETEROGENEOUS MATERIALS

Eliška Janouchová[1,*], Anna Kučerová[1], Jan Sýkora[1]

[1]Faculty of Civil Engineering, Czech Technical University in Prague, Czech Republic,
eliska.janouchova@fsv.cvut.cz, Anna.Kucerova@cvut.cz, jan.sykora.1@fsv.cvut.cz

In order to predict the behaviour of the investigated system in a computational way, the corresponding numerical model has to be properly calibrated. In other words, parameters of the mathematical model of the system have to be estimated as accurately as possible to obtain realistic predictions. Parameter identification of a heterogeneous material model can be formulated as a search for probabilistic description of its parameters providing the distribution of the model response corresponding to the distribution of the observed data.

The underlying uncertainties differ according to whether a source of nondeterminism is irreducible or reducible [1]. Our goal is to quantify aleatory uncertainty which corresponds to real variability of properties in the heterogeneous material, while epistemic uncertainty is supposed to be reduced by any new measurement.

This contribution focuses on two principally different approaches to solving the stochastic inversion problem. The first one is focused on information involved in the experimental data and description of their corresponding joint probability density function based on principal component analysis [2] simultaneously defining the searched joint distribution of the parameters. This method does not allow to distinguish between epistemic and aleatory uncertainties but it does not require any preliminary assumptions about specific type of parameters' density function. On the other side, there is increasingly popular Bayesian inference which enables to estimate the model parameters together with corresponding epistemic uncertainties from indirect experimental measurements [3]. However in case of a heterogeneous material model, the identification procedure has to be able to quantify the aleatory uncertainties capturing the variability of the material properties. By prescribing a specific type of probability distribution with corresponding uncertain statistical moments to the model parameters, the task changes to the identification of these so called hyperparameters of the distribution which can be inferred in Bayesian way [4].

The financial support of the Czech Science Foundation, project No. 16-11473Y, is gratefully acknowledged.

References

[1] Oberkampf, W. L. et al., 2002. Error and uncertainty in modeling and simulation, Reliability Engineering and System Safety 75, pp. 333-357.
[2] Jolliffe, I., 2002. Principal component analysis, 2nd ed. New York: Springer. 487 p. ISBN 03-879-5442-2.
[3] Tarantola, A., 2005. Inverse problem theory and methods for model parameter estimation, Philadelphia, PA: Society for Industrial and Applied Mathematics.
[4] Nagel, J. B., Sudret, B., 2016. A unified framework for multilevel uncertainty quantification in Bayesian inverse problems, Probabilistic Engineering Mechanics, 43, 68-84.

UNCERTAINTY QUANTIFICATION OF AN UNMANNED AERIAL VEHICLE

Henri Dolfen[1], Jolan Wauters[2], Joris Degroote[3], Jan Vierendeels[4]

[1,2,3,4]Department of Flow, Heat and Combustion Mechanics, Ghent University, {henri.dolfen, jolan.wauters, joris.degroote, jan.vierendeels}@ugent.be

I. INTRODUCTION

The research subject is a small, lightweight unmanned aerial vehicle (UAV) made of expanded polypropylene (EPP) foam. During the production process, the foam shrinks. This causes variability in the geometry of the wing, which influences the flight behavior. The goal of this research is demonstrate this through four quantities that characterize flight performance: lift, drag, pitching moment and rolling moment, which are determined using computational fluid dynamics (CFD).

II. METHODOLOGY

An efficient method for uncertainty quantification is found with the Polynomial Chaos method. The investigation is divided in two parts: the first consists of the analysis of a 2D flow problem, namely the flow over a MH60 airfoil. A Monte Carlo method is used as baseline. The results of this investigation are then used to validate a Polynomial Chaos method. The second part is a 3D case, the UAV, and forms the main goal of this work. The validated Polynomial Chaos method is applied on this 3D case.

III. 2D CASE: MH60

The Monte Carlo method exhibits proven convergence that is independent of the dimensionality of the problem. Because of this property, it is considered useful for constructing the baseline case, with which the Polynomial Chaos methods can be compared. A 2D MH60 airfoil is considered, with an uncertainty on the relative thickness. The single input uncertainty is propagated into three output quantities of interest: lift coefficient (C_D), drag coefficient (C_L) and moment coefficient (C_M).

The sampled points are used to validate a Polynomial Chaos method. The main idea on which Polynomial Chaos methods rely is the so-called Polynomial Chaos Expansion (PCE): an infinite sum of polynomials of random variables, multiplied by deterministic coefficients. Two approaches are reviewed to determine the aforementioned truncated sum, namely the Least Squares approach [2] and the quadrature approach [1].

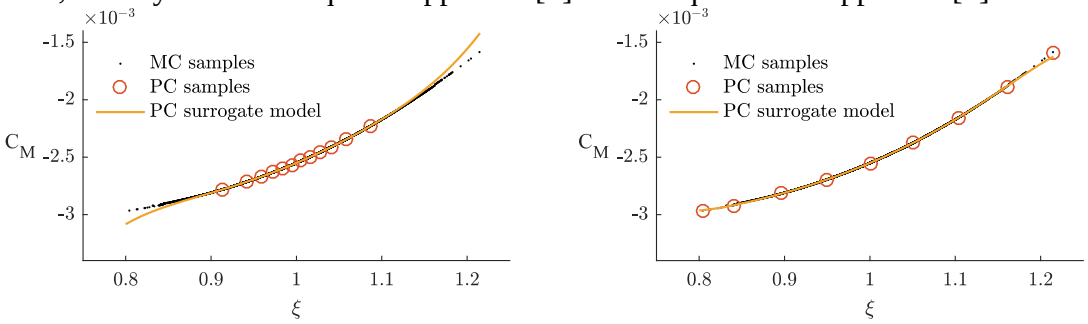


Figure 1. Comparison between Monte Carlo method and Least Squares PC method, 5th order (left) and Gauss–Hermite quadrature PC method, 8th order (right)

Figure 1 shows a comparison of output uncertainty, C_M, for a 5th order Least Squares method and 8th order Gauss–Hermite method. These figures contribute to the conjecture

that the Gauss–Hermite method performs better. The Least Squares method shows a deviation from the simulation data when going to the more extreme values.

IV. 3D CASE: UAV

The two validated Polynomial Chaos methods are applied to the CFD model of the UAV. To have a moderate amount of calculations, it is chosen to only distinguish three input uncertainties: sweep angle, twist angle and shrink of chord, thickness and span. A probability density function (PDF) can then be premised for the input. A normal distribution of which the mean value is based on the comparison between a produced UAV and its mold is presumed for each parameter.

Figure 2 shows the Polynomial Chaos coefficients for the lift force, represented as L_k. A drop of several orders of magnitude can be noticed, going to higher order terms. It is also clearly visible that the low order coefficients of both methods agree, while for higher order polynomials the Least Squares method predicts higher coefficients.

It can also be seen from the first order coefficients, that the volumetric factor (chord, span, thickness) has a positive effect. This is reasonable: a larger wing should create more lift. The twist has a negative coefficient, with a higher magnitude than the volumetric factor. A decreased twist corresponds to a higher local angle of attack (AoA) and thus higher lift. The sweep has the least effect and possesses a negative coefficient as well. This means that decreasing the sweep increases the lift. This can be explained by a higher velocity component normal to the leading edge.

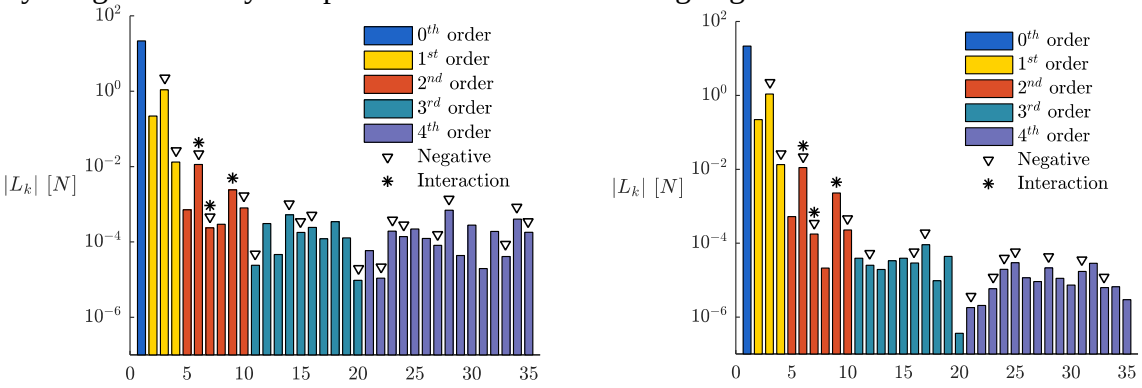


Figure 2. Polynomial Chaos coefficients for the lift force from the Least Squares method, 4th order (left) and from the Gauss–Hermite quadrature method, 4th order (right)

V. CONCLUSION

The uncertainty in the flight behavior and performance of an unmanned aerial vehicle due to its production process has successfully been quantified in an efficient way through the working forces and moments. It is postulated that for this case, the Polynomial Chaos Gauss–Hermite method has more potential, coming at a slightly higher cost.

References

[1] O. P. Le Maître and O. M. Knio, "Spectral Methods for Uncertainty Quantification: With Applications to Computational Fluid Dynamics," Springer Netherlands, 2010.

[2] S. Abraham, M. Raisee, G. Ghorbaniasl, F. Contino and C. Lacor, "A robust and efficient stepwise regression method for building sparse polynomial chaos expansions," *Journal of Computational Physics*, vol. 332, pp. 461-474, 2017.

An immersed variational multiscale solver for large-scale fluid-structure interaction problems in haemodynamics

Liang Yang[1,*], Antonio J Gil[2], Alberto Gambaruto[3]

[1] Department of Earth Science and Engineering, Imperial College London, liang.yang@imperial.ac.uk

[2]Zienkiewicz Centre for Compuatatoinal Engineering, College of Engineering, Swansea University

[3]Department of Mechanical Engineering, Queen's School of Engineering, University of Bristol.

The immersed structural potential method (ISPM) has been used for the haemodynamic simulations [1] and presented in the 'one-fluid' framework [2,3,4]. The ISPM is semi-implicit due to the implicit resolution of the incompressibility constraint. The most time-consuming part is the solution of the Poisson equation within each sub-iteration. Also, due to the explicit formulation of the structure Cauchy stresses, very small time stepping is required [2]. The efficiency of the methodology described above become even more important within the context of the three-dimensional simulations.

Alternatively, a fully explicit algorithm by means of a pseudo-compressibility approach can be used for small density ratio problem, of particular interest in the field of biomechanics. This work presents solving the 'one-fluid' fluid-structure interaction equations in pseudo-compressibility format and algorithm is implemented into the existing pseudo-compressible finite element fluid solver [5]. The fluid solver has been successfully solving over 1 billion unknowns on HPC. The proposed methodology is presented in a fully parallelised framework that allows for the simulation of large-scale three-dimensional haemodynamic problems.

A brief outline of the fundamental equations governing the problem is illustrated here. Consider a general incompressible deformable structure domain Ω_s and an incompressible viscous fluid domain Ω_f in whole domain Ω, in such a way that following relationship is satisfied: $\Omega_s \cup \Omega_f = \Omega;\ \Omega_s \cup \Omega_f = \emptyset$. With a standard non-slip condition on the interface, the FSI coupling the governing equation in 'one-fluid' formulation can be written as:

$$\rho \frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}' + \rho \boldsymbol{g} - \boldsymbol{\nabla} p; \quad \boldsymbol{\nabla} \cdot \boldsymbol{u} = \boldsymbol{0} \tag{1}$$

where the density and deviatoric part of Cauchy stress is defined as $\rho = \rho_f, \boldsymbol{\sigma}' = \boldsymbol{\sigma}'_{\boldsymbol{f}}$ in fluid domain Ω_f, and $\rho = \rho_s, \boldsymbol{\sigma}' = \boldsymbol{\sigma}'_{\boldsymbol{s}}$ in structure domain Ω_s. If we divided the linear momentum equation by ρ_f and re-arranged the equation, we have

$$\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} - \frac{1}{\rho_f} \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}' + \frac{\boldsymbol{\nabla} p}{\rho_f} = \boldsymbol{f} \tag{2}$$

where the volumetric force field $\boldsymbol{f} = \boldsymbol{g}$ in fluid domain Ω_f and $\boldsymbol{f} = \left(1 - \frac{\rho_s}{\rho_f}\right) \frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} + \frac{\rho_s}{\rho_f} \boldsymbol{g}$ in solid domain Ω_s. The pseudo-compressibility replace the divergence free constraint by adding a pseudo-time derivative of the pressure. The continuity equation $\boldsymbol{\nabla} \cdot \boldsymbol{u} = \boldsymbol{0}$ is relaxed as $\partial_{\boldsymbol{t}} p = \epsilon^{-1} \boldsymbol{\nabla} \cdot \boldsymbol{u}$ where ϵ^{-1} is the pseudo compressibility coefficient [5]. Following a standard variational formulation, with suitable functional spaces of test functions $\boldsymbol{v}, q$ for both velocity field $\boldsymbol{u}$ and pressure field p, we can write weak form as

$$\int \partial_t \boldsymbol{u} \cdot \boldsymbol{v} \mathrm{d}\Omega + \int (\boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u}) \cdot \boldsymbol{v} \mathrm{d}\Omega + \int \frac{\boldsymbol{\sigma}'}{\rho_f} : \boldsymbol{\nabla} \boldsymbol{v} \mathrm{d}\Omega - \int \frac{p}{\rho_f} \boldsymbol{\nabla} \cdot \boldsymbol{v} \mathrm{d}\Omega = \int \boldsymbol{f} \cdot \boldsymbol{v} \mathrm{d}\Omega \quad (3)$$

$$\int \partial_t p \, q \, \mathrm{d}\Omega + \epsilon^{-1} \int \boldsymbol{\nabla} \cdot \boldsymbol{u} \, q \, \mathrm{d}\Omega = 0 \quad (4)$$

We have employed the Q1Q1 spatial discretisation for the numerical solution of the variational weak form. The stabilisation and discretisation techniques has been discussed in [5].

The solid stress field $\boldsymbol{\sigma}'_s$ is derived from the stored energy functional and expressed as a function of deformation gradient $\boldsymbol{\sigma}' = f(\boldsymbol{F})$. In this work, we consider a neo-Hookean material model $\boldsymbol{\sigma}' = \boldsymbol{G} J^{-\frac{5}{3}} [\boldsymbol{F}\boldsymbol{F}^{\mathrm{T}} - \frac{1}{3}\mathrm{tr}(\boldsymbol{F}\boldsymbol{F}^{\mathrm{T}})\mathbf{I}$. In fact, the additional internal thermodynamic variables can also be used to further characterise the constitutive law of the structure (including plastic viscoelastic behaviour). Additional conservation of deformation gradient equation is solved as $\frac{\partial \boldsymbol{F}}{\partial t} = \boldsymbol{\nabla} \boldsymbol{u} \boldsymbol{F}$. The introduction of geometric conservation laws has proven to be very efficient circumventing the drawbacks of traditional low order displacement based formulations [3]. The information of the deformation gradient are updates through immersed particles, in the same manner as ISPM, through the interpolation and spreading operator.

Upon the use of a simple fixed point iterative scheme, the coupled FSI equations can be solved to advance from time step n to $n+1$ in an iterative fashion to ensure the complete coupling of the fluid and solid. By computing a residual norm based upon the difference between the deviatoric Cauchy stress tensor $\boldsymbol{\sigma}'_s$ in two successive iterations k and $k+1$, a convergence criterion can be easilly estabilished. With each sub-iteration, we solve the conservation of linear momentum equation, conservation of the deformation gradient, and the conservation of the mass, and the interface tracking problem.

$$\boldsymbol{u}_{i+1}^{n+1} = \boldsymbol{u}^n - \Delta t \ \mathrm{RHS}(\boldsymbol{u}^n, p^n, \boldsymbol{\sigma}'_s(\boldsymbol{F}_i^{n+1})) \quad \text{conservation of linear momentum} \quad (5)$$

$$\partial_t \boldsymbol{F}_{i+1}^{n+1} = \boldsymbol{\nabla} \boldsymbol{u}_{i+1}^{n+1} \boldsymbol{F}_i^{n+1} \quad \text{conservation of deformation gradient} \quad (6)$$

$$p_{i+1}^{n+1} = p^n - \Delta t \ \mathrm{RHS}(\boldsymbol{u}^n) \quad \text{conservation of mass} \quad (7)$$

$$\mathrm{D}\boldsymbol{X}_{i+1}^{n+1}/\mathrm{D}t = \boldsymbol{u}_{i+1}^{n+1} \quad \text{geometric tracking} \quad (8)$$

References

[1] Gil, A.J., Carreno, A.A., Bonet, J., 2012. The immersed structural potential method for haemodynamic applications. Journal of Computational Physics, 229.22: 8613-8641.

[2] Yang, L., 2015. An immersed computational framework for multiphase fluid-structure interaction. Ph.D. thesis, Swansea University.

[3] Yang, L, Gil, A.J., Carreno, A.A., Bonet, J., 2017. Unified one-fluid formulation for incompressible flexible solids and multiphase flows: application to hydrodynamics using the Immersed Structrual Potential Method (ISPM). (In press).

[4] Yang, L, Carreno, A.A., Gil, A.J., Bonet, J., 2014. An immersed structural potential framework for incompressible flexible/rigid/multi-phase flow interaction. Proceeding of 22nd UK Conference of the Association for Computational Mechanics in Engineering.

[5] Yang, L., Badia, S., Codina, R., 2016. A pseudo-compressible variational multiscale solver for turbulent incompressible flows. Computational Mechanics, 58(6), 1051-1069.

MULTISCALE MIXED-MODE FAILURE CRITERION AND TRACTION-SEPARATION RELATION FOR COMPOSITE MATERIALS

Sergio Turteltaub[1,*], Niels van Hoorn[2], Wim Westbroek[3] , Christian Hirsh[4]

[1]Faculty of Aerospace Engineering, Delft University of Technology, The Netherlands, S.R.Turteltaub@tudelft.nl

[2]Faculty of Aerospace Engineering, Delft University of Technology, The Netherlands, Niels.van.Hoorn@nlr.nl

[3]Faculty of Aerospace Engineering, Delft University of Technology, The Netherlands, W.Westbroek@student.tudelft.nl

[4]Faculty of Mechanical Science and Engineering, TU Dresden, Germany, Christian.Hirsch2@mailbox.tu-dresden.de

Failure analysis of composite materials, such as fiber-reinforced laminates, requires establishing a relevant connection between the macroscopic response behavior and the microscale fracture mechanisms of the material. The growth of cracks observable at larger length scales (i.e., macrocracks) is controlled by the distinct fracture mechanism that may be activated at the microscale, such as matrix cracking, fiber cracking, debonding or combinations thereof [1]. In turn, the nucleation and growth of microcracks depend on the applied loads, the microstructural characteristics (e.g., volume fractions), the fracture properties of the constituents and their bonding strength and adhesion fracture energy.

A multiscale numerical homogenization framework based on a crack-averaged Hill-Mandel condition is developed in order to establish the existence of a representative volume element in the presence of localized crack. Expressions for the effective crack opening and effective traction are established from this analysis, which includes the use of periodic boundary conditions for arbitrarily-oriented cracks and the notion of an effective crack that contains information about localization and is nominally independent of periodic replicas.

An effective nucleation criterion and traction-separation relation (cohesive law) for fiber-reinforced composites is subsequently developed with the aim of incorporating microscopic fracture mechanisms under various mode mixity loading conditions in a unified, simple expression that is useful for analysis and design purposes. The relation is based on an extensive parametric study carried out to correlate the constituents' fracture properties, their adhesion strength and microstructural characteristics to the macroscopic fracture properties (see Figure 1)

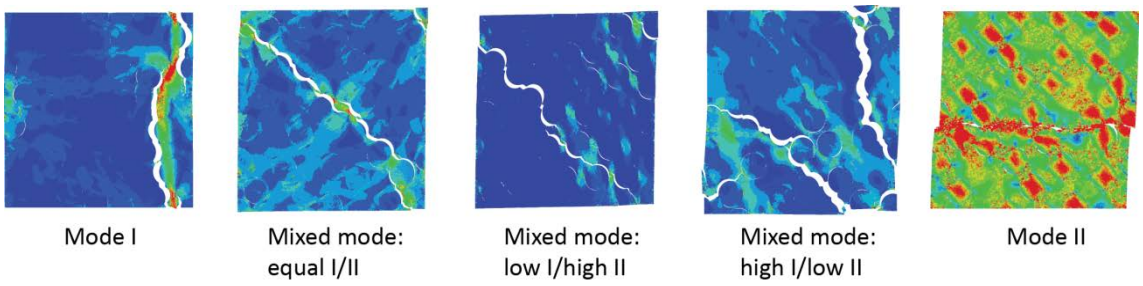


Figure 1. Distinct load cases for a given microstructural configuration and material properties

In this approach, the computational effort is concentrated in an a-priori calibration of the macroscopic traction-separation relations for arbitrary loading conditions and for a wide range of combinations of material properties. These relations can subsequently be used in single-scale macroscopic simulations for general loading conditions and for composites of distinct characteristics, which is useful for design purposes. The overall computational gain is achieved by reducing the total number of microscale simulations since these are replaced by effective traction-separation relations. The procedure is a computationally-attractive alternative to fully-coupled multiscale simulations [2,3].

References

[1] Ponnusami, S.A., Turteltaub, S., van der Zwaag, S., 2015, Cohesive-zone modelling of crack nucleation and propagation in particulate composites, Eng. Frac. Mech., 149, 170-190.

[2] Remmers, JC, Gutierrez, MA, de Borst, R., 2010, Computational homogenization for adhesive and cohesive failure in quasi-brittle solids, Int. J. Num. Meth. Eng. 83(8-9):1155-1179

[3] Bosco, E.; Kouznetsova, V. G.; Geers, M. G. D., 2015, Multi-scale computational homogenization-localization for propagating discontinuities using X-FEM, Int. J. Num. Meth. Eng. 102 (3-4) SI 496-527

FINITE ELEMENT MODELING OF NANOSTRUCTURED PIEZOELECTRIC COMPOSITES AND USES IN ULTRASOUND APPLICATIONS: EXAMPLE OF TRANSDUCER WITH PLANO-CONCAVE FACE

Anna Nasedkina [1,*], Andrey Nasedkin [2], Andrey Rybyanets [3]

[1] Institute of Mathematics, Mechanics & Computer Science, Southern Federal University, 344090 Rostov-on-Don, Russia, email: nasedkina@math.sfedu.ru

[2] Institute of Mathematics, Mechanics & Computer Science, Southern Federal University, 344090 Rostov-on-Don, Russia, email: nasedkin@math.sfedu.ru

[3] Physics Research Institute, Southern Federal University, 344090 Rostov-on-Don, Russia, email: arybyanets@gmail.com

In the recent time an increased interest has been observed to the investigations of piezocomposite materials that exhibit very effective properties for many practical applications. Thus, new nanostructured piezocomposite materials have a range of important advantages, such as the possibilities of controllable variation of the functional characteristics within a wide range, the ultra-low mechanical quality factor, and the large electromechanical anisotropy.

The first part of our research concerns direct finite element modeling of piezoelectric mixture two-phase composites. The proposed technique is based on the models of micro- and nanoscale materials with surface effects, the effective moduli method, modeling of representative volumes and the use of finite element technology [1]. As particular case we investigate the porous piezoceramic materials. For these materials we use the special models of representative volume of porous material with different types of connectivity, take into account for the heterogeneity of piezoceramic polarization near the pores [2-5] and surface effects on the boundaries of nanosized pores. Here, we apply the generalized Gurtin-Murdoch model of surface effects with special conditions for stresses and electric flux discontinuities at the borders between piezoelectric material and pores [6, 7].

In second part to increase the efficiency of electro-mechanical transformation it is proposed to use the circular transducer from nanostructured porous piezoceramics in which one of its end surfaces has a plano-concave shape. We suppose that this transducer will have greater flexibility for bending deformation and, as a consequence, will have large effective piezomoduli.

In the computational experiments the plane-concave transducers with electrode face plates made from nanostructured porous piezoceramics PCR-1 have been examined. The effective thickness piezomodule d_{33} was obtained in quasi-static tests with a force F applied at the center of the top plane surface. The transducer was placed on the foundation, leaning on the flat part of its bottom end surface of the plano-concave form. Under the action of the force F the transducer was deformed, and due to the piezoelectric effect the electric charges Q have appeared on the electrodes. The effective thickness piezomodule was defined as the ratio of the induced charge to the applied force: $(d_{33})^{\text{eff}}=Q/F$.

For the proposed plano-concave disk circular transducer we were carried out the finite element modeling using ANSYS. We have built solid and finite element models of the

considered transducer in the axisymmetric statement. Developed programs allowed to calculate the effective thickness piezomoduli for different geometrical and physico-mechanical input data and for different size of porosity under static and harmonic analyses. As it was found, the appropriate selection of the quasi-static values of the transducer quality factor is very important for correlation between calculating and experimental results for low-frequency vibrations.

Since the experimental and computation results have shown a good agreement for the test samples, that it allows to predict the effective properties of a plano-concave transducer for various input data by using the appropriate computer calculations. Naturally, the effective piezoelectric moduli increase with decreasing of disk height and with increasing of concavity radius. So, for the certain input data we have obtained an increase of the effective thickness piezomodule compared with the piezomodule of dense material a hundreds time, that it opens up the various possibilities of using the new circular piezoelectric transducer for different applications.

The reported study was funded by RFBR according to the research project 16-01-00785.

References

[1] Nasedkin, A.V., Kornievsky, A.S., 2017. Finite element modeling and computer design of anisotropic elastic porous composites with surface. In: Methods of wave dynamics and mechanics of composites for analysis of microstructured materials and metamaterials. Ser. Advanced Structured Materials, Vol. 59, M.A. Sumbatyan (Ed.). Springer, Singapore, Ch. 6, 107-122.

[2] Nasedkin, A., Rybjanets, A., Kushkuley, L., Eshel, Y., Tasker, R., 2005. Different approaches to finite element modelling of effective moduli of porous piezoceramics with 3-3 (3-0) connectivity. Proc. 2005 IEEE Ultrason. Symp., Rotterdam, Sept. 18 -21, 2005, 1648-1651.

[3] Lupeiko, T.G., Nasedkin, A.V., Nasedkina, A.A., 2011. Mathematical modeling and optimization of piezoelectric generator of nanostructured piezoceramic. Proc. IC-EpsMsO – 4th Int. Conf. Experiments/Process/System Modeling/Simulation/ Optimization, Athens, Greece, 6-9 July, 2011. Ed. D.T. Tsahalis. University of Patras, LFME. Vol. 2, 358-365.

[4] Nasedkin, A.V., Shevtsova, M.S., 2011. Improved finite element approaches for modeling of porous piezocomposite materials with different connectivity. In: Ferroelectrics and superconductors: Properties and applications. Ed. I.A. Parinov. Nova Science Publishers, N.-Y., Ch.7, 231-254.

[5] Nasedkin, A.V., Shevtsova, M.S., 2013. Multiscale computer simulation of piezoelectric devices with elements from porous piezoceramics. In: Physics and mechanics of new materials and their applications. Eds. I.A. Parinov and S.-H. Chang. Nova Science Publishers, N.-Y., Ch. 16, 185-202.

[6] Eremeyev, V.A., Nasedkin, A.V., 2017. Mathematical models and finite element approaches for nanosized piezoelectric bodies with uncoulped and coupled surface effects. In: Methods of wave dynamics and mechanics of composites for analysis of microstructured materials and metamaterials. Ser. Advanced Structured Materials, Vol. 59, M.A. Sumbatyan (Ed.). Springer, Singapore, Ch. 1, 1-18.

[7] Nasedkin, A., 2017. Size-dependent models of multiferroic materials with surface effects. Ferroelectrics 509, 57-63.

APPLICATION OF NON-INTRUSIVE INVERSE PROBLEM IN CIVIL ENGINEERING

Jan Havelka[1,*], Jan Sykora[2], Anna Kucerova[3]

[1]Czech Technical University in Prague, Department of Mechanics, jan.havelka.1@fsv.cvut.cz

[2]Czech Technical University in Prague, Department of Mechanics, jan.sykora.1@fsv.cvut.cz

[3]Czech Technical University in Prague, Department of Mechanics, anna.kucerova@cvut.cz

In specific fields of research such as preservation of historical structures, medical imaging, material science, geophysics and others, it is of particular interest to perform only a non-intrusive boundary measurement. The idea is to obtain a comprehensive information about the material properties inside the domain under consideration while maintaining the test sample intact. This contribution is focused on such problems i.e. synthesizing a physical model of interest with a boundary inverse techniques. The forward model is represented by diffusion based models with Finite Element (FE) discretisation and the parameters are subsequently recovered using a modified Calderón problem principles which is numerically solved by a regularised Gauss-Newton method. We provide a basic framework, implementation details and modification of general constrains originally derived for a standard setup of Calderón problem. The proposed model setup was numerically verified for various domains, load conditions and material field distributions. Both steady-state and time dependent cases are studied.

References

[1] Calderón, A.P., 2006, On an inverse boundary value problem, Computational & Applied Mathematics, **25**,133 – 138

[2] Holder, D.S., 2004, Electrical Impedance Tomography: Methods, History and Applications, Taylor & Francis.

[3] Vauhkonen, M., Lionheart, W.R.B., Heikkinen, L.M., Vauhkonen, P.J. and Kaipio, J.P., 2001, A MATLAB package for the EIDORS project to reconstruct two-dimensional EIT images, Physiological Measurement, 22(1), 107.

[4] Sylvester, J. and Uhlmann, G., 1987, A Global Uniqueness Theorem for an Inverse Boundary Value Problem, Annals of Mathematics, 125(1), 153-169.

[5] Nachman, A.I., 1996, Global Uniqueness for a Two-Dimensional Inverse Boundary Value Problem, Annals of Mathematics, 143(1), 71-96.

[6] Langer, R.E. (1933), An inverse problem in differential equations, Bulletin of the American Mathematical Society, 39(10), 814-820.

Reaction-diffusion-chemotaxis model on uncertainty parameters

Ana Paula Pintado Wyse[1], Antônio José Boness dos Santos[1] ,Juarez dos Santos Azevedo[2,*]

[1] PPGMMC- UFPB, 58051-900, João Pessoa–PB, Brazil

[2]CETEC-UFRB, Centro, 44380-000, Cruz das Almas-BA, Brazil

In this work, we propose a model described by a system of stochastic differential equations of the reaction-diffusion-chemotaxis type that describes the spread and interaction between wild and transgenic mosquitoes, where the transgenic population has a reduced CO_2 detection capacity, which makes it difficult to blood orientation and therefore reduces the bitting rate on humans. In this approach, the underlying random fields, such as diffusion coefficient, are modeled as second-order stochastic processes and are expanded using Karhunen-Loève expansion on Monte Carlo method. For this purpose, the model was solved numerically using the sequential operator splitting technique, with the reactive part of the system solved by the fourth-order Runge-Kutta and the diffusive-chemotaxis part by the Crank-Nicolson method. The numerical simulations obtained attest to the consistency of the model with the assumptions adopted.

References

[1] J.D.Murray. Mathematical Biology I: An introduction, volume 17. Springer, New York, 2002.

[2] E. F. Keller and L. A. Segel. Initiation of slime mold aggregation viewed as an instability. J. Journal of Theoret. Biol, 26:399–415, 1970.

[3] E. F. Keller and L. A. Segel. Model for chemotaxis. J. Journal of Theoret. Biol, 30:225–234, 1971.

HEURISTIC TECHNIQUE FOR DESIGN OF ROBUST EXPERIMENTS BASED ON GLOBAL SENSITIVITY

Anna Kučerová[1,*], Jan Sýkora[1], Eliška Janouchová[1], Daniela Jarušková[1]

[1]Faculty of Civil Engineering, Czech Technical University in Prague, Czech Republic,
anna.kucerova@cvut.cz, jan.sykora@fsv.cvut.cz, eliska.janouchova@fsv.cvut.cz,
daniela.jaruskova@cvut.cz

Recent developments in the field of uncertainty quantification open more possibilities to simulate the nonlinear systems with uncertain input parameters. Nowadays, they also allow for determination of relevant input uncertainties through inverse analysis of noisy data. As a next step in terms of computational complexity come problems belonging to the field of optimisation under uncertainty.Their complexity arises generally from exhaustive probabilistic computations (simulation of a system or inverse analysis) which need to be performed repeatedly within complex optimisation process. One example of such a complex problem is design of robust and optimal experiments taking into account uncertainties in input parameters (noise variables).

In our contribution we concentrate on the design of experiment problem described in Ruffio et al. [1]. The aim of the experiment modelled on 2D squared domain is to provide the most precise information about thermophysical material properties: volumetric thermal capacity and the conductivities in the two principal directions, while considering uncertainties a) in the constant heat flux prescribed on two edges, b) in the position of three measuring sensors and c) in the values of temperature measured in 60 time steps. Considering such noise variables and linear non-stationary model of heat transfer, the corresponding inverse analysis cannot be solved analytically due to the nonlinear relationship between measured values of temperature on one side and identified material properties or noise variables on the other side.

Assuming one realisation of such an experiment, where material properties attained some fixed albeit unknown value, probably the most general solution of the probabilistic inverse analysis covers repeated deterministic solution of least square problem for Monte Carlo sampling of noise variables. As a result one obtains the sampled distribution of material parameter estimates. Within the process of experiment design, the goal is often to minimise the variance of this estimated distribution. The process of design optimisation thus requires repeated solution probabilistic inverse analysis for any change of design variables. When the optimality criterion based on estimated variances is complex function as in our case, some robust optimisation algorithm (e.g. some evolutionary algorithm) is needed and probabilistic solution of underlying inverse analysis has to be performed in thousands or millions of repetitions. Moreover, if the experiment design is supposed to be not only optimal, but also robust, it has to consider that unknown identified material parameters may attain any value from some interval or prior distribution. The probabilistic solution of inverse analysis thus has to be performed not only once at each iteration of optimisation algorithm but for instance several times for some sampled values of material parameters.

In order to overcome the described computational complexity, Ruffio et al. [1] propose a solution based on linearisation of the model. It allows to replace the probabilistic solution of inverse analysis by a fast analytical solution providing an explicit formula for computing covariance matrix of material parameter estimates. The robustness of the design is then provided by evaluating the analytical solution for a set of samples of material properties and optimisation is governed by evolutionary algorithm. However, in Jarušková and Kučerová [2] it is demonstrated that the employed linearisation of the model significantly distorts the result of the probabilistic inverse analysis.

In our contribution we replace the linearisation by a higher order polynomial approximation of the model response in order to reduce the approximation error. Such an approximation unfortunately does not provide an analytical solution of the probabilistic inverse analysis. Nevertheless, it provides an analytical formulation of Sobol indices expressing the global sensitivity of model response to identified material properties as well as to noise variables [3]. The traditional optimality criterion based on covariance matrix of material parameter estimates is here replaced by analogue criterion based on global sensitivity matrix. The method can be thus viewed as heuristic, because the optimality in terms of sensitivity does not guarantee optimality w.r.t. estimated variance. Nevertheless, we demonstrate that the proposed approach provides better experiment designs than the method based on linearisation on the described example. Moreover, global sensitivity indices already include the information about the feasible interval or prior distribution of identified material properties and thus the criterion is robust and does not need any further sampling in the space of identified quantities. Therefore, the proposed method allows for better handling of model nonlinearity and design robustness at the price of heuristic optimality criterion based on global sensitivity.

The financial support of the Czech Science Foundation, project No. 15-07299S, is gratefully acknowledged.

References

[1] Ruffio, E. and D. Saury and D. Petit. Robust experiment design for the estimation of thermophysical parameters using stochastic algorithms. International Journal of Heat and Mass Transfer, 55(11-12):2901–2915, 2012.

[2] Jarušková, D. and A. Kučerová: Estimation of thermophysical parameters revisited from the point of view of nonlinear regression with random parameters. *International Journal of Heat and Mass Transfer*, 106, 135-141, 2017.

[3] Blatman, G and Sudret, B. Efficient computation of global sensitivity indices using sparse polynomial chaos expansions. Reliability Engineering and System Safety, 95(11):1216–1229, 2010.

DIGITAL ROCK PHYSICS: SEGMENTATION COMPARISON FOR A CARBONATE ROCK

A. Islam[1], T. Faisal[1], M. S. Jouini[2], M. Sassi[1]

[1]Masdar Institute of Science and Technology, P.O. Box 54224, Abu Dhabi, U.A.E.

[2]The Petroleum Institute of Abu Dhabi, PO Box 2533, Um al Nar, Abu Dhabi, United Arab Emirates

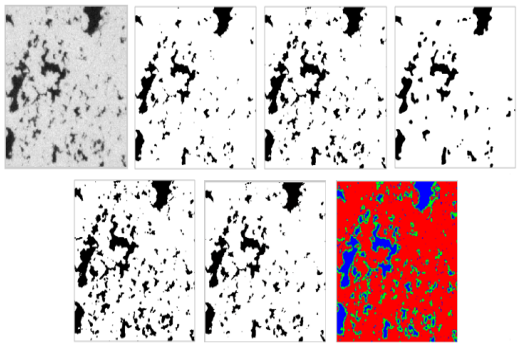
Abstract Conventional rock physics analyses are crucial in the field of oil and gas as they allow for the characterization and management of reservoir production. Digital Rock Physics (DRP) is an emerging field that helps determine rock properties from images. The main workflow of DRP involves three steps; image acquisition, image segmentation and numerical computation. In this work, a systematic study was conducted where different segmentation techniques were applied to determine their effect on porosity and permeability values of a carbonate rock sample.
Keywords-Digital Rock Physics; Image Segmentation; Carbonates

I. INTRODUCTION: Digital Rock Physics (DRP) [1]–[5] combines the recent advances in imaging technology with numerical simulations to digitally determine properties quickly without risking damage to the core plug.

The main workflow of DRP involves three steps; image acquisition, image segmentation and numerical computations[6], [7]. Image acquisition can be done via any of the available imaging technologies such as X-ray computed tomography (XCT) that allow for the non-invasive imaging of the core plug to resolutions down to the micron range[8]. Image segmentation is the separation of the image into discrete phases – usually the pore space as well as one or more solid phase depending on the type of mineralogy of the sample. The segmentation stage is crucial for DRP as it could alter the results of numerical simulations. In this work, a systematic study was conducted where different segmentation techniques were applied to determine their effect on porosity and permeability values.

II. METHODOLOGY: Images of a carbonate rock were acquired from a 0.5 inch diameter cylindrical core sample at a resolution of 13.24 micrometer using a micro-CT. Even though the image dataset acquired was of the size of 1004x1024x1995voxels, for the purpose of this study, a cubic subvolume of size 300^3 voxel was extracted. Following that, five segmentation algorithms were studied;

1. Global thresholding. In this method, two threshold values were selected to denote the minimum and maximum pore space that could be determined visually.
2. Otsu's algorithm [9], which is an automated global thresholding algorithm that minimizes the weighted sum of variances of the two classes (background and object).
3. K-means algorithm [10] that defines clusters based on the peaks of the histogram of the image and then to partition the data points in such a way that minimizes the sum of the squared distance to the center of the cluster[10].
4. Watershed segmentation as run on Avizo [11].
5. Watershed segmentation with top hat.



Segmentation	Total Porosity	Effective porosity	Permeability (D)
Interactive Thresholding – Low	0.0977	0.0372	0.134
Interactive Thresholding - High	0.138	0.113	0.592
Watershed	0.103	0.039	0.2125
Tophat and watershed	0.167	0.153	1.7116
Otsu	0.138	0.113	0.5954
K-means	0.0845	No connection	No connection

Figure 1. [From left to right] (a) Original Image (b) Minimum thresholding (c) Maximum thresholding (d) Watershed (e) Watershed and Tophat (f) Otsu (g) K-means

III. RESULTS: As shown in the table of figure 1, segmentation results show that the total porosity, effective porosity and permeability can vary greatly depending on the segmentation type used. While Otsu's algorithm gave similar results to the manually selected thresholding technique on the high side, the rest fell into two extremes; with k-means, manual (low) threshold and watershed on the lower end, and watershed with top hat on the upper end. The range of permeability spans from "no connectivity" to a 1.71 Darcy permeability.

IV. CONCLUSIONS

As can be seen from the results of this study, the choice of segmentation technique is important in determining the properties of rocks using Digital Rock Physics tools. That is why it is recommended that protocols using Digital Rock Physics are run alongside experiments for validation.

V. REFERENCES

[1] C. H. Arns, M. A. Knackstedt, W. V. Pinczewski, and E. J. Garboczi, "Computation of linear elastic properties from microtomographic images : Methodology and agreement between theory and experiment," vol. 67, no. 5, pp. 1396–1405, 2002.

[2] A. Kameda and J. Dvorkin, "To see a rock in a grain of sand," *Lead. Edge*, vol. 23, no. 8, pp. 790–792, 2004.

[3] C. H. Arns, M. A. Knackstedt, W. V. Pinczewski, and N. Martys, "Virtual permeametry on microtomographic images," *J. Pet. Sci. Eng.*, vol. 45, no. 1–2, pp. 41–46, 2004.

[4] A. Sakellariou, C. H. Arns, A. P. Sheppard, R. M. Sok, H. Averdunk, A. Limaye, A. C. Jones, T. J. Senden, and M. A. Knackstedt, "Developing a virtual materials laboratory," *Mater. Today*, vol. 10, no. 12, pp. 44–51, 2007.

[5] J. T. Fredrich, a. a. DiGiovanni, and D. R. Noble, "Predicting macroscopic transport properties using microscopic image data," *J. Geophys. Res.*, vol. 111, no. B3, p. B03201, 2006.

[6] H. Andrä, N. Combaret, J. Dvorkin, E. Glatt, J. Han, M. Kabel, Y. Keehm, F. Krzikalla, M. Lee, C. Madonna, M. Marsh, T. Mukerji, E. H. Saenger, R. Sain, N. Saxena, S. Ricker, A. Wiegmann, and X. Zhan, "Digital rock physics benchmarks—Part I: Imaging and segmentation," *Comput. Geosci.*, vol. 50, pp. 25–32, Jan. 2013.

[7] H. Andrä, N. Combaret, J. Dvorkin, E. Glatt, J. Han, M. Kabel, Y. Keehm, F. Krzikalla, M. Lee, C. Madonna, M. Marsh, T. Mukerji, E. H. Saenger, R. Sain, N. Saxena, S. Ricker, A. Wiegmann, and X. Zhan, "Digital rock physics benchmarks—part II: Computing effective properties," *Comput. Geosci.*, vol. 50, pp. 33–43, Jan. 2013.

[8] F. Fusseis, X. Xiao, C. Schrank, and F. De Carlo, "A brief guide to synchrotron radiation-based microtomography in (structural) geology and rock mechanics," *J. Struct. Geol.*, vol. 65, pp. 1–16, 2014.

[9] N. Otsu, "A Tlreshold Selection Method from Gray-Level Histograms," *IEEE Trans. Syst. man Cybern.*, vol. SMC-9, no. 1, pp. 62–66, 1979.

[10] N. Salman, "Image Segmentation Based on Watershed and Edge Detection Techniques," *Int. Arab J. Inf. Technol.*, vol. 3, no. 2, pp. 104–110, 2006.

[11] FEI, "Avizo User Guide." [Online]. Available:

http://www.vsg3d.com/sites/default/files/AvizoUsersGuide.pdf. [Accessed: 01-Jan-2014].

TIME-FREQUENCY SOLUTION OF SEISMIC STABILITY OF ROCK SLOPES

Gang Fan[1]; Li-Min Zhangb[2]; Jian-Jing Zhang[3]

[1]Department of Civil and Environmental Engineering, The Hong Kong University of Science and Technology, Hong Kong, P. R. China; e-mail: fangang@ust.hk.

[2]Department of Civil and Environmental Engineering, The Hong Kong University of Science and Technology, Hong Kong, P. R. China.

[3]School of Civil Engineering, Southwest Jiaotong University; Chengdu, Sichuan, P. R. China.

Abstract: In current methods for seismic stability analysis of rock slopes, the time-frequency-amplitude characteristics of the earthquake waves are not considered. A time-frequency solution for calculating the seismic safety factor of rock slopes is derived in this paper. The Hilbert-Huang transform (HHT) signal processing technique is adopted to identify the time-frequency-amplitude characteristics of the earthquake waves in the time-frequency domain. Then a time-frequency method for computing instantaneous seismic safety factor of rock slopes considering the time-frequency-amplitude characteristics of the earthquake waves simultaneously, is proposed. Shaking table test examples are conducted to illustrate the application of the proposed time-frequency analysis method. The instantaneous seismic safety factors of typical bedding and counter-bedding rock slopes are calculated based on the time-frequency analysis method proposed in this research.

Keywords: Time-frequency analysis; seismic response; slope stability; HHT; rock slope; shaking table test.

REVERSE MAPPING METHOD FOR COMPLEX POLYMER SYSTEMS

Jakub Krajniak[1*], Sudharsan Pandiyan[2], Zidan Zhang[2], Dirk Roose[1], Erik Nies[2], Giovanni Samaey[1]

[1]KU Leuven, Department of Computer Science, Celestijnenlaan~200A, 3001~Leuven, Belgium
[2]KU Leuven, Division of Polymer Chemistry and Materials, Department of Chemistry, Celestijnenlaan 200F, 3001 Leuven, Belgium

We present a comprehensive approach for reverse mapping of complex polymer systems in which the connectivity is created by the simulation of chemical reactions at the coarse-grained scale. Within the work, we use a recently developed generic adaptive reverse mapping procedure[1], that we adapt to handle the varying connectivity structure resulting from the chemical reactions. As the examples, we apply the method to reverse map four different systems: a three-component epoxy network, a trimethylol melamine network, a hyperbranched polymer and polyethylene terephthalate systems. We validate the fine-grained structure by comparing the radial distribution functions with respect to the control parameter. Moreover, in the case of epoxy network and melamine, we also perform tensile-test experiment and examine the resulting Young's modulus. In all cases, we show how the properties of the reverse mapped systems depend on the control parameters. In general, we see that the results are relatively insensitive to the control parameter and the resulting atomistic systems are stable.

References

[1] Krajniak J, Pandiyan S, Nies E, Samaey G, 2016 Adaptive Resolution Method for Reverse Mapping of Polymers from Coarse-Grained to Atomistic Descriptions, Journal of Chemical Theory and Computation

ON THE PREDICTIVE ABILITY OF A CONTINUUM DAMAGE MODEL THROUGH AN HOMOGENIZATION-BASED MULTI-SCALE MODEL

Bernardo P. Ferreira[1], Francisco M. Andrade Pires[1], Igor A. Rodrigues Lopes[1]

[1]Department of Mechanical Engineering, Faculty of Engineering, University of Porto,
bpferreira@fe.up.pt, fpires@fe.up.pt, ilopes@fe.up.pt

Abstract

Over recent years, the modeling of heterogenous multi-phase materials has been a topic of extensive research and increasing interest by the scientific community. Among other approaches, computational homogenization-based multi-scale modeling has emerged as an effective way to relate the macroscopic behaviour of materials with their underlying heterogeneous microstructure by continuous interchange of information between scales. Under the key assumption of the principle of separation of scales, the hierarchically coupled multi-scale finite element method is based on the nested solution of two coupled boundary value problems: (i) at the macroscale, where the material's macroscopic response is sought, and (ii) at the microscale, where computations are conducted over representative volume elements in order to account for microstructural phenomena in the macroscopic response, through an homogenization procedure.

Ductile fracture by void nucleation, growth and coalescence is one of the main failure mechanisms of structural metallic alloys. Although this subject has received attention for more than 50 years, striving for the development of better alloys and for more reliable damage models is continuously bringing up new challenges. In fact, since the pioneering micromechanical void growth model proposed by Gurson [1], several continuum damage models, either micromechanicaly or phenomenologicaly based, were developed, accounting for increasingly complex aspects, namely void geometry evolution, plastic anisotropy and stress state dependence. Due to the direct link between scales, computational homogenization-based multi-scale modeling has the potential to become assess, develop and optimize continuum damage models.

In the present contribution, a first order homogenization-based multi-scale model [2,3] is employed to critically assess the predictive ability of the widely known Gurson's void growth model [1]. To this end, simulations of three-dimensional specimens, under low and high (positive) stress triaxiality regimes, are conducted with both models, and the results obtained at the macro and at the microscale are compared. In what concerns the multi-scale model, the appropriate modeling of representative volume elements, with single and multiple voids, allows a clear insight of the damage evolution in the material microstructure over monotonic deformation paths.

References

[1] Gurson, A. L. (1977). Continuum theory of ductile rupture by void nucleation and growth: Part I – yield criteria and flow rules for porous ductile media. Journal of Engineering Materials and Technology, 99.

[2] de Souza Neto, E. A. And Feijóo, R. A. (2006). Variational foundations of multi-scale constitutive models of solid: Small and large strain kinematical formulation. Technical report, LNCC R&D.

[3] Reis, F. J. P. (2014). Multi-scale Modeling and Analysis of Heterogeneous Solids at Finite Strains. PhD thesis, Faculty of Engineering, University of Porto.

MULTI-SCALE CONSTITUTIVE MODELLING OF MULTIPHASE ALLOYS

M.V. de Carvalho[1,*], D. de Bortoli[2], F.A. Andrade Pires[3]

[1]Faculty of Engineering of the University of Porto, Portugal, mvcarvalho@fe.up.pt

[2]INEGI – Institute of Science and Innovation in Mechanical and Industrial Engineering, Portugal, ddbortoli@fe.up.pt

[3]Faculty of Engineering of the University of Porto, Portugal, fpires@fe.up.pt

Multiphase alloys, such as TRIP (*transformation induced plasticity*) and dual-phase steels, enjoy considerable technological importance. These materials have favourable mechanical properties such as a combination of high yield strength and elongation at failure. The computational modelling of their constitutive behaviour poses a number of challenges stemming from complex interactions between multiple deformation mechanisms in the microscopic scale, such as plastic slip and martensitic phase transformations.

Over the last decades, a variety of phenomenological and micromechanical constitutive models have been proposed in the literature, accounting for the major features of their macroscopic behaviour (for instance, [1, 2]). Nevertheless, these usually involve a large number of material parameters that require experimental calibration, limiting their predictiveness and generalisability. In this context, multi-scale models are a natural fit due to their ability to both capture the fine-scale crystalline features and connect them to the macroscopic, engineering scale. The overall material behaviour can thus be directly obtained from modelling the multiple constituent phases – namely, slip in FCC or BCC lattices, for the ferrite, martensite and stable austenite phases, and FCC-to-BCC phase transformations, for the meta-stable austenite crystallites.

For slip plasticity, robust algorithms are required to handle the non-smooth yield functions and the determination of an active system set under general loading scenarios. Moreover, the presence of linearly dependent systems can result in non-unique solutions for the plastic multipliers. The frequently employed rate-dependent regularisations [3] circumvent these difficulties but make the resulting equations extremely stiff in the limit of vanishing rate-sensitivity parameters, leading to convergence issues in the stress integration algorithm. Here, a fully implicit rate-independent formulation, using the volume-preserving exponential map [4] and strategies such as sub-stepping and an active system selection procedure based on [5–7], is employed.

Additionally, the effect of mechanically-induced martensitic transformations is introduced using a recently proposed generalisation of Patel and Cohen's [8] energy-based criterion. The resulting model also includes coupling effects with the evolution of austenite slip activity, bearing many similarities with the aforementioned crystal plasticity models. Thus, analogous computational difficulties arise and are tackled similarly.

As previously discussed, the macroscopic behaviour of multi-phase crystalline materials is intrinsically related to their complex microstructure. In order to study that connection, the above material models are incorporated into a large strains fully implicit, RVE- based

multi-scale finite element code. Both RVE homogenisation and fully coupled (FE^2) analyses are performed to study the influence of microstructural parameters on the resulting behaviour for materials of interest for which experimental data is available, such as metastable austenitic stainless steels and TRIP steels.

References

[1] J. B. Leblond. "Mathematical Modelling of Transformation Plasticity in Steels II: Coupling with Strain Hardening Phenomena". In: *International Journal of Plasticity* 5.6 (1989).

[2] M. Cherkaoui, M. Berveiller, and X. Lemoine. "Couplings between Plasticity and Martensitic Phase Transformation: Overall Behavior of Polycrystalline TRIP Steels". In: *International Journal of Plasticity* 16 (10–11 2000).

[3] R. J. Asaro and A. Needleman. "Overview No. 42: Texture Development and Strain Hardening in Rate Dependent Polycrystals". In: *Acta Metallurgica* 33.6 (1985).

[4] C. Miehe. "Exponential Map Algorithm for Stress Updates in Anisotropic Multiplicative Elastoplasticity for Single Crystals". In: *International Journal for Numerical Methods in Engineering* 39.19 (1996).

[5] L. Anand and M. Kothari. "A Computational Procedure for Rate-Independent Crystal Plasticity". In: *Journal of the Mechanics and Physics of Solids* 44.4 (1996).

[6] R. I. Borja and J. R. Wren. "Discrete Micromechanics of Elastoplastic Crystals". In: *International Journal for Numerical Methods in Engineering* 36.22 (1993).

[7] H. K. Akpama, M. B. Bettaieb, and F. Abed-Meraim. "Numerical Integration of Rate-Independent BCC Single Crystal Plasticity Models: Comparative Study of Two Classes of Numerical Algorithms". In: *International Journal for Numerical Methods in Engineering* 108.5 (2016).

[8] J. R. Patel and M. Cohen. "Criterion for the Action of Applied Stress in the Martensitic Transformation". In: *Acta Metallurgica* 1.5 (1953).

Damage of heterogeneous composite material: from the fibres to structural level

P. Bussetta[1,*], R. Tavares[1,2,3], F. Otero[1], P. Camanho[1, 2] and N. Correia[1]

[1]INEGI - Composite Materials and Structures
Institute of Mechanical Engineering and Industrial Management, Porto 4200-465, Portugal
pbussetta@inegi.up.pt; fotero@inegi.up.pt; ncorreia@inegi.up.pt
[2]DEMEC, Faculdade de Engenharia, Universidade do Porto, 4200-465, Porto- Portugal
pcamanho@fe.up.pt
[3]AMADE, Polytechnic School, University of Girona, Campus Montilivi s/n, 17071 Girona, Spain
em10140@fe.up.pt

One of the main problems of the composite materials reinforced with continuous fibres (carbon or glass) is the low value of the failure strain and the fragile fracture behaviour. Composite materials can be hybridised to have a pseudo-ductile behaviour. The hybrid composite material here considered is a composite material reinforced with continuous fibres of different diameters and/or material properties. This work deals with the integration of the micro scale model into the meso scale one. A numerical micro scale model of the tensile fracture in the fibre direction based on the Spring Element Model (SEM) is presented [1]. The SEM is an efficient computational approach to simulate tensile failure of unidirectional composites. The model originally was based on the assembly of periodic packages of fibre and matrix spring elements. Later, an extension to consider random distribution of fibres and hybrid composites was proposed [2] . The SEM consists of longitudinal spring elements, which represent the fibres, connected by transverse spring elements representing the matrix. The matrix contribution in the fibre direction is disregarded, which is a commonly accepted hypothesis for UD polymer composites. Therefore, only the matrix shear contribution in the tensile failure process is represented through shear transverse elements. In the proposed approach, the composite is modelled thanks to truss and membrane elements at the meso scale level [3] . Moreover, the truss element behaviour is obtained through the proposed micro scale model. In addition, the membrane element takes in consideration the important behaviour, e.g. shear, that the multiscale element truss are not able to consider. Finally, the presented multiscale formulation is used to model the fracture behaviour of the composite materials at the structure level.

References

[1] Okabe, T., Sekine, H., Ishii, K., Nishikawa, K., Takeda, N., 2005. Numerical method for failure simulation of unidirectional fiber-reinforced composites with spring element model, Composites Science and Technology 65 (6) 921-933. doi: 10.1016/j.compscitech.2004.10.030

[2] Tavares, R. P., Otero, F., Turon, A., Camanho, P. P., 2017. Effective simulation of the mechanics of longitudinal tensile failure of unidirectional polymer composites, International Journal of Fracture (Submit).

[3] Harrison, P., Gomes, R., Curado-Correia, N., 2013. Press forming a 0/90 cross-ply advanced ther-moplastic composite using the double-dome benchmark geometry. Composites Part A: Applied Science and Manufacturing, 54, 56–69. doi: 10.1016/j.compositesa.2013.06.014.

EFFICIENT SURROGATE MODELS FOR RELIABILITY ANALYSIS OF SYSTEMS WITH FUZZY RANDOM VARIABLES

Muhannad Aldosary[1,*], C.F.Li[2], D.R.J. Owen[3]

[1]Swansea University,Swansea,UK., 716663@swansea.ac.uk

[2]Swansea University, Swansea, UK., c.f.li@swansea.ac.uk

[3]Swansea University, Swansea, UK., d.r.j.owen@swansea.ac.uk

Abstract: Nowadays, uncertainty propagation in complex engineering is intrinsic to physical processes and simulation methods. The epistemic uncertainty (lack of knowledge) alongside aleatory uncertainty (natural variability), which are represented the major sources of uncertainty in the input variables, are included in this paper. The mix of these two sources of uncertainties is often referred to as imprecise probabilities. These uncertainties of the input variables are modelled by fuzzy random variables for estimating the bounds on the reliability of structural systems. Due to the complexity of the computer simulations by using fuzzy random variables, the meta-models are used throughout this paper. Sparse polynomial chaos expansions or Kriging meta-model is used to surrogate the exact computational model and, hence, to facilitate the uncertainty quantification analysis. The accuracy and efficiency of the proposed method are demonstrated through several numerical examples. In addition the comparison between the two meta-models are also given. The results show that the meta-model approaches give an accurate estimation for the membership function of the failure probability by using a small number of evaluations of the exact computational model.

Keywords: structure reliability, fuzzy random variable, polynomial chaos expansion, Kriging, meta-model.

1. Introduction

Although many sources of uncertainty may exist, they may be classified into two major groups, aleatory and epistemic. The aleatory uncertainty refers to the inherent uncertainty due to probabilistic variability and usually is modelled by random variables. While the epistemic uncertainty is caused by the lack of knowledge. The modelling of the epistemic uncertainty still represents a challenging topic [1]. The best solution to include the epistemic uncertainty is by using the fuzzy set theory. In this paper, incomplete knowledge about the distribution parameters is modelled using fuzzy random variables. Therefore, the reliability assessment is also expressed in terms of fuzzy numbers. In the literature there are several methods to solve the fuzzy reliability system. The α-cut approach [2] is one of the most commonly used approaches to estimate the fuzziness in the systems. A variety of methods can used to obtain the bounds of the failure probability for each α-cut. One of these methods proposed to use the search algorithm [3] combined with MCS to determine the bounds of the response. However, all these methods are involved with MCS, which lead to time consuming. In order to reduce the computational costs and to make uncertainty quantification analyses tractable, this paper is providing two surrogate models. The first one is non-intrusive sparse polynomial chaos and the second one is Kriging meta-model.

2. Meta-model of systems with fuzzy random variables

Operationally, a fuzzy random variable is a random variable taking fuzzy values. A fuzzy variable is represented as a set of interval variables via the membership function. Considering the probability space (Ω, f, P), a membership function $\pi_{\tilde{A}}(\omega) \in [0,1]$ indicates the degree of possibility that an elementary event ω belongs to a set $\tilde{A}$. In other words, it can be interpreted as a distribution of uncertainty. So, any fuzzy set can be expressed by a set of pairs as follow:

$$\tilde{A} = \{(x, \pi_{\tilde{A}}(x)) | x \in \Omega; \pi_{\tilde{A}}(x) \in [0,1]\} \quad (1)$$

A fuzzy realization is assigned to each event ω in Ω, see Fig.(1). The bounds of failure probability at each α-cut can be evaluated by using PCE or Kriging mehods, see Fig. (2). The main features of the meta-model algorithms corresponding to type of the fuzzy random variable are shown in Table (1). Due to the restriction in abstract length, more results will be presented in the conference.

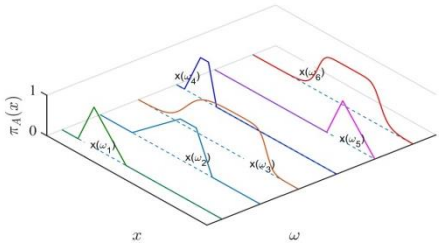


Fig.(1) Membership function for fuzzy Rv.

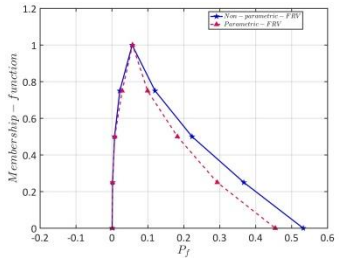


Fig.(2) Membership function for failure probability.

Table 1. Comparison between the fuzzy meta-model methods

		Non-Parametric Fuzzy	Parametric Fuzzy
PCE	Input	$\underline{F}_X$, $\overline{F}_X$:(upper and lower CDF)	$F_X(\boldsymbol{x}\|\boldsymbol{\rho}),\ \boldsymbol{\rho} \in D_P$
	Meta-model	$G(\boldsymbol{X}),\ \underline{G}(\boldsymbol{U}),\ \overline{G}(\boldsymbol{U})$: limit state fun.	$G^{(aug)}(\boldsymbol{V})$
	Dimensionality	$\|\boldsymbol{X}\| = \|\boldsymbol{U}\| = M$	$\|\boldsymbol{V}\| = \|\boldsymbol{X}\| + \|\boldsymbol{P}\| = M + \|\boldsymbol{P}\|$
Kriging	Input	$\underline{F}_X$, $\overline{F}_X$	$F_X(\boldsymbol{x}\|\boldsymbol{\rho}),\ \boldsymbol{\rho} \in D_P$
	Meta-model	$G(\boldsymbol{X}),\ \underline{G}(\boldsymbol{U}),\ \overline{G}(\boldsymbol{U})$	$G^{(Kriging)}(\boldsymbol{x})$
	Dimensionality	$\|\boldsymbol{X}\| = \|\boldsymbol{U}\| = M$	$\|\boldsymbol{P}\|,\ \|\boldsymbol{X}\| = M$

References

[1] Hanss, M. & Turrin, S. (2010), A fuzzy based approach to comprehensive modeling and analysis of systems with epistemic uncertainties. Structural Safety, 32(6),433–41.

[2] Möller, B. &Beer,M. (2004), Fuzzy-Randomness-Uncertainty in Civil Engineering and Computational Mechanics, Springer-Verlag.

[3] Möller, B. & Beer,M. (2008), Engineering computation under uncertainty—capabilities of non-traditional models, Computers and Structures, 86, 1024–41.

[4] Schobi, R. and B. Sudret, Uncertainty propagation of p-boxes using sparse polynomial chaos expansions. Journal of Computational Physics, 2017. 339: p. 307-327.

STATISTICAL RECONSTRUCTION OF HETEROGENEOUS MATERIALS

S.Q. Cui[1,*], C.F.Li[2] , D.R.J. Owen[3]

[1]College of Engineering, Swansea University, Swansea, UK, s.cui.714627@swansea.ac.uk

[2]College of Engineering, Swansea University, Swansea, UK, c.f.li@swansea.ac.uk

[3]College of Engineering, Swansea University, Swansea, UK, d.r.j.owen@swansea.ac.uk

It is well known that the randomness exists everywhere. When people do the numericial simulations, the critial thing is to make the simulations as close as possible to the reality so as to get the most accurate results. To this end, the randomness should be taken into consideration, and this is also exactly what more and more researchers and scientists did. In nature, it is impossible to find out two material samples with the same microstructure, even they all belong to the same type of material. Thus, for the calculations (or the predictions) of the equivalent macroscopic properties of materials, or the studies of mechanical responses of materials, the large amount of the numerical samples with random microstructures is required.

The most challenging problem about microstructure reconstruction is how to efficiently achieve a realistic three-dimensional computational model with a highly accurate representation of the random heterogeneous material. The three-dimensional microstructure of media can be directly reconstructed by using a large number of sectioning and imaging, but these 3D imaging techniques are often costing and have restrictions in sample size and shape. Therefore, based on the statistical information obtained from several two-dimensional slices (thin sections) of a random medium or experimental images, it is desirable to reconstruct the full three-dimensional medium that matches the statistical information of the original microstructure, enabling computational and theoretical prediction of the macroscale properties (e.g., permeability, conductivity and elastic moduli). This kind of technique can also be used to efficiently generate a large amount of equivalent two-dimensional microstructures based on several (or even one) reference two-dimensional sample(s), or efficiently generate two-dimensional microstructures of any size or boundary shape.

If we need to deduce the statistical information from the scanning image of the reference sample, the scanning images still need to be processed further. For most of statistical reconstruction algorithms, all types of random media should be represented as n-phase media, which can be described by the corresponding indicator function $I(\boldsymbol{x}), \forall x \in D$, D is the spatial domain of the sample, that is,

$$I(\boldsymbol{x}) = \begin{cases} 0, & \boldsymbol{x} \in \mathcal{V}_1 \\ 1, & \boldsymbol{x} \in \mathcal{V}_2 \\ \cdots & \cdots \\ n-1, & \boldsymbol{x} \in \mathcal{V}_n \end{cases} \tag{1}$$

where $\mathcal{V}_i$ is the region occupied by phase i(i=1,2,…,n).

In this work, a comprehensive comparison study of the statistical reconstruction algorithms is done. All commonly used statistical reconstruction algorithms are implemented, and classified into several groups based on four aspects, i.e. the type of

preserved statistical information, the source of preserved statistical information, the processing scope and the phase number. The performances of these statistical reconstruction algorithms are then compared by using four types of cases, which are two-dimensional two-phase media reconstructions, three-dimensional two-phase media reconstrucitons, two-dimensional multi-phase media reconstructions and three-dimensional multi-phase media reconstrucitons. Moreover, three factors are discussed for the performance analysis of these reconstruction algorithms, which are accuracy, efficiency and applicability. Some of the results are shown below,

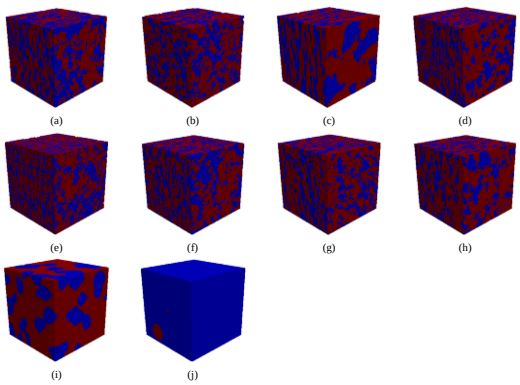
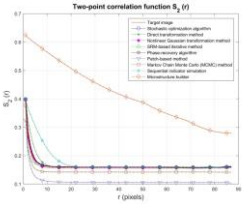


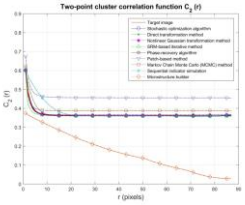
Figure 1. Image size 100*100*100 pixels, (a) the reference sample; (b-j) the reconstructions via SA, DT, NGT, CC, MCMC, PR, SRM, SIS and MB respectively, and the corresponding CPU times are 40368s, 0.19s, 2.22s, 159.81s, 4373.96s, 64.65s, 1361.72s, 60071s and 111s respectively.



(a1)

The Sum of Squared Residuals			
Stochastic optimization algorithm	2.67E-04	Patch-based Method	2.60E-01
Direct transformation method	7.97E-03	Markov Chain Monte Carlo (MCMC) method	3.35E-02
Nonlinear Gaussian transformation method	2.13E-03	Sequential indicator simulation	9.46E-02
SRM-based iterative method	7.17E-03	Microstructure builder	6.24E+00
Phase-recovery algorithm	5.47E-04		

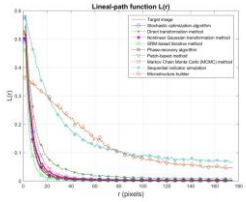
(b1)



(a2)

The Sum of Squared Residuals			
Stochastic optimization algorithm	4.42E-04	Patch-based Method	7.64E-01
Direct transformation method	7.99E-03	Markov Chain Monte Carlo (MCMC) method	5.77E-02
Nonlinear Gaussian transformation method	2.31E-03	Sequential indicator simulation	9.50E-02
SRM-based iterative method	7.20E-03	Microstructure builder	4.25E+00
Phase-recovery algorithm	5.54E-04		

(b2)



(a3)

Stochastic optimization algorithm	4.10E-03	Patch-based Method	4.05E-02
Direct transformation method	1.22E-01	Markov Chain Monte Carlo (MCMC) method	1.70E-02
Nonlinear Gaussian transformation method	1.00E-02	Sequential indicator simulation	3.48E+00
SRM-based iterative method	1.03E-01	Microstructure builder	3.26E+00
Phase-recovery algorithm	1.61E-02		

(b3)

Figure 2. Accuracy analysis for the cases in Figure 1

In Fig. 1, the reference sample in (a) is reproduced by using different algorithms. The CPU times for these involved algorithms are listed as well. In Figure 2, the accuracies of these realizations are compared by using two-point correlation functions (Fig.2.a1), two-point cluster correlation functions (Fig.2.a2) and lineal-path functions (Fig.2.a3). Due to the restriction in abstract length, more results will be presented in the conference.

References

[1] Yeong, C. L. Y. and Torquato, S., 1998. Reconstructing random media. PHYSICAL REVIEW E, vol 57, no.1.

[2] Li, D.S., 2014. Review of Structure Representation and Reconstruction on Mesoscale and Microscale, The Minerals, Metals & Materials Society, 16, No. 3.

[3] Xu, H. Y., Li, Y., Brinson, C., 2014. A Descriptor-Based Design Methodology for Developing Heterogeneous Microstructural Heterogeneous Microstructural, Journal of Mechanical Design, Vol. 136, 051007

[4] Feng, J.W., Li, C.F., Owen, D.R.J., 2014. Statistical reconstruction of two-phase random media, Computers and Structures 137, 78-92

[5] Tahmasebi, P., & Sahimi, M. (2013). Cross-Correlation Function for Accurate Reconstruction of Heterogeneous Media. Physical Review Letters, 110(7). doi: 10.1103/PhysRevLett.110.078002

Polynomial normal transformation function and its application in structural reliability analysis

Jinsheng Wang[1,*], C.F. Li[2], D.R.J. Owen[3]

[1]Swansea University, Swansea, UK., 844051@swansea.ac.uk

[2]Swansea University, Swansea, UK., c.f.li@swansea.ac.uk

[3]Swansea University, Swansea, UK., d.r.j.owen@swansea.ac.uk

In practical engineering problems, it is somehow inevitable that uncertainties may involved in during the service lifetime of a structure. Therefore, accurate approaches to assess the uncertainties present in engineering systems, i.e. load conditions, material properties, structural dimensions and environmental factors, are required in the process of structural design and analysis, and thus has led to the development of numerous uncertainty quantification methods. Uncertainty quantification pursues many general objectives connected to quantify the effects of the uncertain input parameters of a model on its outputs. As one of the classical methods of uncertainty quantification using the probability theory, a fundamental problem in structural reliability analysis is the evaluation of failure probability of a structural system under a specific threshold, which can be formulated as a multidimensional integral:

$$P_f = \text{Prob}[\text{g(X)} \le 0] = \int_{g(\text{X})\le 0} f_X(x)dX \qquad (1)$$

where $X = [X_1, X_2, \cdots, X_n]^T$ is a n-dimensional random vector represents uncertain quantities; P_f is the failure probability; $g(X)$ is the performance function defined such that $g(X) \le 0$ denotes the failure domain and $g(X) > 0$ the safe domain, the boundary between safe and failure domain is known as the limit state surface, i.e. $g(X) = 0$; $f_X(x)$ is the joint probability density function (PDF) of the random vector X .

Although the definition and formulation of structural reliability as shown in Eq. (1) is quite simple, the exact evaluation by direct integration is often intractable if not impossible because the dimension of the integral is usually high, $g(X)$ is of complicated shape and sometimes even expressed implicitly. These difficulties has led to the development of various reliability approximation methods, such as first-order reliability method (FORM) , second-order reliability method (SORM), Monte Carlo simulation (MCS), importance sampling methods, directional simulation methods and others [1-3]. It is quite often that most of the aforementioned methods are originally developed on the assumption that all random variables involved are normally distributed. When it comes to non-normal random variables, normal transformation techniques are usually applied, among which Rosenblatt transformation, Nataf transformation and polynomial transformation are some of the well known techniques. Of interested here in this study is the polynomial transformation method, where the second-order and third-order polynomial normal transformation functions are commonly used and can be respectively formulated as [4-5]:

$$x_s = a_1 + a_2 u + a_3 u^2 \qquad (2)$$

$$x_s = a_1 + a_2 u + a_3 u^2 + a_4 u^3 \qquad (3)$$

where x_s is the original standardized non-normal random variable, u is the standard normal random variable, and a_0, a_1, a_2, a_3 are the deterministic polynomial coefficients to be determined. Four different methods to determine the polynomial coefficients are investigated by Chen [6].

Herein the present study, several methods for structural reliability analysis are proposed based on the polynomial normal transformation function. A third-moment reliability index is derived from the inverse transformation of Eq. (2) and thus a new second-order third-moment reliability analysis method is developed by incorporating the first three statistical moments of the parabolic approximation of performance function. Some of the numerical comparison results are illustrated in Fig. 1 and Table. 1.

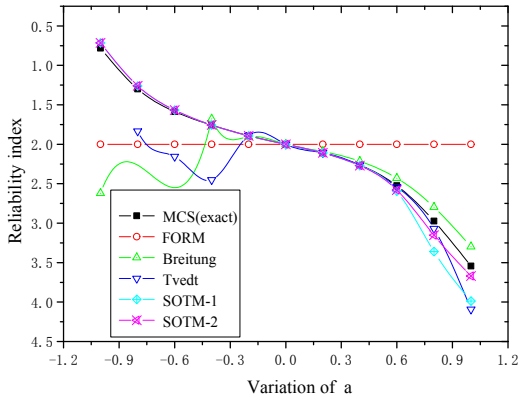


Figure 1. Comparison results for example 1

Table 1. Comparison results for example 2

Methods		Reliability index	Probability of failure	Error
MCS		1.5966	0.05518	---
FORM		1.9710	0.02436	55.9%
SORM	Breitung	1.5917	0.05573	1.0%
	Tvedt	1.4505	0.07346	33.1%
SOTM-1		1.5954	0.05531	0.2%
SOTM-2		1.5953	0.05532	0.3%

Moreover, the existing third-order polynomial normal transformation function expressed in Eq. (3) is only feasible for independent random variables, it is further extended to deal with problems involving correlated random variables. Through this procedure, the normal transformation can be accomplished using only the first four statistical moments of the correlated random variables, without needing to know the probability density function as required in Rosenblatt transformation and Nataf transformation. It is in this regard that the presented technique is especially attractive when only samples of the random variables are available. More details regarding the accuracy and applicability of the proposed approaches will be given in the presentation.

References

[1] H.O. Madsen, S. Krenk and N.C. Lind, Methods of Structural Safety, Prentile-Hall, Englewood Cliffs, N.J., 1986;

[2] Schuëller G I, Stix R. A critical appraisal of methods to determine failure probabilities . Structural Safety, 1987, 4(4):293-309.

[3] Nie J, Ellingwood B R. Directional methods for structural reliability analysis. Structural Safety, 2000, 22(3):233-249.

[4] Zhao Y G, Ono T. Third-Moment Standardization for Structural Reliability Analysis. Journal of Structural Engineering, 2000, 126(6):724-732.

[5] Zhao Y G, Asce M, Lu Z H. Fourth-moment standardization for structural reliability assessment. Journal of Structural Engineering, 2007, 133(7):916-924.

[6] Chen X, Tung Y K. Investigation of polynomial normal transform. Structural Safety, 2003, 25(4):423-445.Lee, E.H., 1969. Elastic-plastic Deformation at Finite Strains. Journal of Applied Mechanics 36, 1–6.