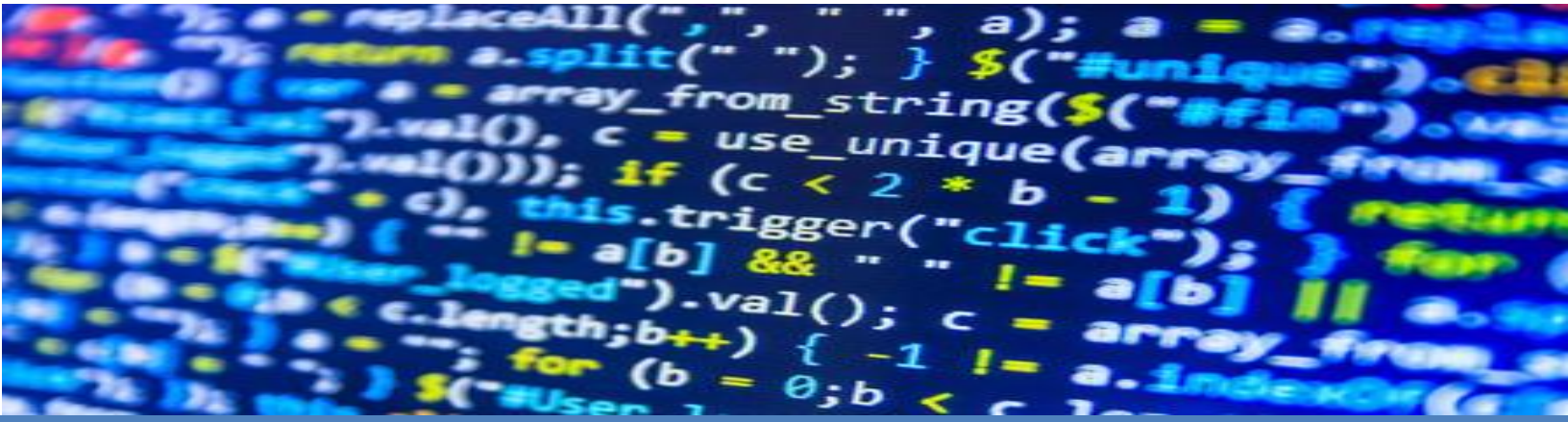


COMPUTATIONAL METHODS IN MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Porto | 15 -16 - 17 July

@Fundação Dr. António Cupertino de Miranda

Avenida da Boavista, 4245
Porto

Chairpersons

CHAIRPERSONS

Dr. F.M. Andrade Pires
Department of Mechanical Engineering (DEMec)
Faculty of Engineering, University of Porto (FEUP)
Phone: +351 22 5083479,
fpires@fe.up.pt

Dr. Chenfeng Li
College of Engineering, Swansea University
Phone: +44 (1792) 602256,
c.f.li@swansea.ac.uk

LOCAL ORGANIZING COMMITTEE

Carla Monteiro
Department of Mechanical Engineering (DEMec)
Faculty of Engineering, University of Porto (FEUP
monteiro@fe.up.pt

About

The development of multi-scale, multi-uncertainty and multi-physics models has received significant attention over the last two decades. New mathematical formulations and numerical solution strategies allied to the increase in computational power/cost ratio have fostered a dramatic growth in this rapidly expanding field. Research activity in this area has been devoted to the development and combination of different analytic tools (homogenization, asymptotic analysis) and computational methods (parallel computing, stochastic analysis, code coupling) for application in fields as diverse as metal processing, composite material, oil & gas development, fuel cell technology and biomedical tissue engineering, etc. Such developments have played a central role in the understanding of the interaction among multi-physics and multi-uncertainty phenomena taking place at multiple scales in space and time.

In the most general format, the ECCOMAS Thematic Conference CM4P targets the latest advances in the modelling of in multi-scale, multi-uncertainty and multi-physics problems, and welcomes the following (not exhaustive) research topics:

- Computational homogenization and multi-scale modelling
- Stochastic modelling, probabilistic engineering, reliability and risk assessment
- Computer simulation of multi-physics processes/systems

WIFI NETWORK NAME: CCONGRESSOS

PROGRAM

July 15th	
08:30- 09:20	Registration
09:20 - 09:30	Welcome Remarks
09:30 - 10:20	**Plenary Session 1** **CHARACTERIZATION OF MAGNETO-ELECTRIC COMPOSITES: AN ALGORITHMIC SCALE-BRIDGING SCHEME** **Jörg Schröder** | Institute of Mechanics, Civil engineering – Duisberg – Essen University | Germany
10:20 - 10:40	**Coffee-Break**
Session Chairs:	@Auditorium: @Room A: @Room B:
10:40 – 11:00	Presentation 1.1 **Paper 5** Irina Tezaur: **The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics** Sandia National Laboratories **@Auditorium** Presentation 1.2 **Paper 18** Michele Serpilli: **On modeling interfaces in composite with multi-physic coupling** Università Politecnica delle Marche **@Room A** Presentation 1.3 **Paper 43** Bert Mortier: **Diffusion-Kinetic Monte Carlo Methods for Neutral Transport in Plasma Edge Simulations of Nuclear Fusion Reactors** KU Leuven **@Room B**
11:00 - 11:20	Presentation 1.4 **Paper 41** Wan-Chun Chuang: **Simulation Model for Single unit Warpage of Shadow moire in Flip-Chip Process** National Sun Yat-sen Universit **@Auditorium** Presentation 1.5 **Paper 37** Marco Delucia: **Development of a modified Voronoi's tesselation algorithm for the determination of the effective properties of cork-based composites** Laboratoire I2M, Arts et Métiers ParisTech **@Room A** Presentation 1.6 **Paper 44** Dmytro Pivovarov: **Development of a simple ergodic stochastic representative volume element for heterogeneous materials with random geometry of microstructure_LTM**, FAU Erlangen-Nuremberg **Room B**

11:20 - 11:40	Presentation 1.7 **Paper 25**_Emanuela Bosco: **A computational multi-physics model to predict the chemo-mechanical degradation of historical oil paintings**_Eindhoven University of Technology**@Auditorium** Presentation 1.8 **Paper 250**_Pawel Holobut: **Assessment of the Size of the Representative Volume Element of Random Heterogeneous Materials**_Institute of Fundamental Technological Research, Polish Academy of Sciences_**@Room A** Presentation 1.9 **Paper 231**_Anna Matveeva: **Virtual material characteriazation across scales and physics: case studies**_Siemens Industry Software NV **Room B**
11:40 - 12:00	Presentation 1.10 **Paper 230**_Szymon Nosewicz: **Multiscale prediction of powder properties during pressure-assisted sintering**_Institute of Fundamental Technological Research Polish Academy of Sciences**@Auditorium** Presentation 1.11 **Paper 221**_Avraham Seifert_**On the universality of the Strouhal law for High Reynolds number bluff bodies with flow control**_Tel Aviv University_**@Room A** Presentation 1.13 **Paper 31**_ Lori Graham-Brady_**Fragment size characterization for granular flow in highly damaged ceramics**_ Johns Hopkins University_**@Room B**
12:00 - 12:20	Presentation 1.14 **Paper 201**_Younes Ya Aoues_**System time-variant reliability-based structural design optimization of deteriorated truss bridges**_Normandie Université, INSA Rouen France_**@Auditorium** Presentation 1.15 **Paper 20**_ Katharina Kremer_ **Sub-Modeling Approach to Investigate the Cracking Behavior of Reinforced Concrete Structures Considering Polymorphic Uncertainty**_Ruhr-Universitaet Bochum_**@Room A** Presentation 1.16 **Paper 28**_ Martin Doskar_ **Reduced-order Modelling Scheme for Problems with Fully Resolved Microstructures Generated by Generalized Periodic Unit Cells**_ Czech Technical University in Prague_**@Room B**
12:20 - 13:30	**Lunch Break**
Afternoon	

13:30 - 14:20	**Plenary Session 2** **BRIDGING THE GAP: A JOINT AUSTRO-CHINESE RESEARCH PROJECT ON MULTISCALE MODELING – STRUCTURAL ANALYSIS – EXPERIMENTS** **Prof. Herbert Mang |** Institute for Mechanics of Materials and Structures, TU Wien | Austria
Session Chairs:	@Auditorium: @Room A: @Room B:
14:40 – 15:00	Presentation 1.17 **Paper 246**_ Bahram Haddadi Sisakht_ **Increased Modelling Demands by Moving from Resolved to Unresolved Simulation of Heterogeneous Reactive Systems**_ TU Wien – ICEBE **@Auditorium** Presentation 1.18 **Paper 234**_ Mijo Nikolic_ **Modelling of shear bands in fluid saturated poroplastic solids with embedded strong discontinuities**_ University of Split, Faculty of Civil Engineering, Architecture and Geodesy_Croatia_**@Room A** Presentation 1.19 **Paper 42**_ Christian Gierden_**Efficient and accurate two-scale FE-FFT-based prediction of polycrystalline material behavior at finite strains**_ RWTH Aachen University_**@Room B**
15:00 - 15:20	Presentation 1.20 **Paper 220**_Pedro Prates_ **Machine Learning-based Approach for Predicting Defects under Uncertainty in Sheet Metal Forming Processes**_ University of Coimbra**@Auditorium** Presentation 1.21 **Paper 242**_Caetano Miranda_ **Nanoscience applied to oil and gas technologies: a multiscale computational approach**_ Universidade de Sao Paulo_**@Room A** Presentation 1.22 **Paper 226**_ Xiangling Gao_**Multi-scale Numerical Simulation of Reinforced Concrete Framed Structure**_ Tongji University_**@Room B**

15:20 - 15:40	Presentation 1.23 Paper **218** Mohsen Ayoobi_**Data-Drive Approaches in Predicting Premixed Reactive Flow** Wayne State University_ USA**@Auditorium** Presentation 1.24 **Paper 241**_ Christian Jordan_ **New Method for Numerical Calibration of a Rotary Kiln Model** - A Multiscale Approach _ TU Wien/Institute of Chemical Engineering **@Room A** Presentation 1.25 **Paper 213**_Lu Hai_ **A phase-field damage model with micro inertial effect for dynamic failure of quasi-brittle materials_**Tongji University_**@Room B**
15:40 – 16:00	Coffee Break
16:00- 16:20	Presentation 1.26 **Paper 265**_ Mohamadreza Afrasiabi_**A Thermo-Mechanically Coupled Cutting Simulation of Ti-6Al-4V Using Advanced Meshless Methods**_ ETH Zurich**@Auditorium** Presentation 1.27 **Paper 223**_ Shuai Guo_**Robust Flame Frequency Response Identification via a Multi-Fidelity Approach**_ Technical University Munich_**@Room A** Presentation 1.28 **Paper 27**_Linda J. Bolay **Degradation of Lithium-Ion Batteries in Aerospace**_German Aerospace Cente_**@Room B**
16:20 - 16:40	Presentation 1.29_ **Paper 235**_ Ruofan Gao_**Comparison of Two New Methods for Fatigue Reliability_Analysis**_Tongji University_China**@Auditorium** Presentation 1.30 **Paper 26**_ Emanuela Bosco_**A coupled chemo-mechanical model for biogenic sulfide corrosion in concrete sewer pipes**_ Eindhoven University of Technology_ Netherlands_**@Room A** Presentation 1.31_**Paper 8**_Christoph Pohl_**Pore Water State in Heated Concrete - Comparing a Numerical Model to NMR Measurements**_Bundesanstalt für Materialforschung und –prüfung Germany_**@Room B**
17:00	**Departure from the Conference´s venue**
17:30	**Welcome Session: Visit to Port Wine Cellars followed by Port Wine Tasting**

July 16th	
09:00 - 09:50	**Plenary Session 3** **HYBRID TWINS: ADAPTING TO MULTI-UNCERTAIN EVOLVING ENVIRONMENTS** **Prof.Francisco Chinesta | ENSAM ParisTech | France**
09:50 - 10:40	**Plenary Session 4** **COMPUTATION-BASED DESIGN POLYMER COMPOSITE FOR SHOCK WAVE ENERGY ATTENUATION** **Zhuo Zhuang** | School of Aerospace Engineering, Tsinghua University, Beijing | China
10:40 - 11:00	Coffee Break
Session Chairs:	@Auditorium: @Room A: @Room B:
11:00 - 11:20	Presentation 2.1 **Paper 244**_De-Cheng Feng_**Stochastic Finite Element Analysis of U-Shaped RC Shear Wall with a Novel Random Field Modeling Strategy for Open Thin-Walled Structural Members_** Southeast University China**@Auditorium** Presentation 2.2 **Paper 264**_ Lorraine Aparecida Silva_ **Simulation of adhesive squeeze flow using smoothed particle hydrodynamics**_Institut Clément Ader France_**@Room A** Presentation 2.3 **Paper 256**_Bernardo Proença Ferreira_**A Finite-Strain Elasto-Viscoplastic Model for Rubber Toughened Glassy Polymers: Formulation and Validation**_Faculty of Engineering of the University of Porto_Portugal**@Room B**

11:20 - 11:40	Presentation 2.4 **Paper 237**_Reza Ghaffari_**A Vibrational study of graphene sheets, carbon nanotubes, and nanocones**_Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University Germany**@Auditorium** Presentation 2.5 **Paper 248**_Prem Ratan Mohan Ram_**Approximation of frequency response functions with the multi-element generalised polynomial chaos method**_TU Braunschwei Germany_**@Room A** Presentation 2.6 **Paper 11**_Witold Ogierman_ **Computationally efficient homogenization for modeling of nonlinear functionally graded materials**_ Silesian University of Technology Poland_**@Room B**
11:40- 12:00	Presentation 2.7 **Paper 269**_ Florent Grotto_**Multiphysical simulation of aluminum panels' behaviour hit by lightning strikes**_ICA / ISAE-SUPAERO France**@Auditorium** Presentation 2.8 **Paper 215**_Ye Feng **Two-scale phase field modeling of damage and fracture for disordered media**_Tongji University China_**@Room A** Presentation 2.9 **Paper 253**_Igor Lopes_**A Fully Second-Order Homogenisation Model for the Analysis of Multi-Phase Materials at Finite Strains**_ University of Porto_Faculty of Engineering Portugal_**@Room B**
12:00-12:20	Presentation 2.10 **Paper 266**_ Boussad Abbes_**Multiphysics Simulation of Laser Metal Deposition Manufacturing Process Using a Meshless Method**_University of Reims Champagne-Ardenne | France**@Auditorium** Presentation 2.11 **Paper 232**_Robin Kamenicky_**Heat transfer partitioning models for nucleate boiling**_University of Strathclyde | United Kingdom_**@Room A** Presentation 2.12 **Paper 262**_Dmitry Grebennikov_**Computational methods for hybrid multiscale modelling in immunology**_Marchuk Institute of Numerical Mathematics of the Russian Academy of Sciences |Russian Federation_**@Room B**
12:20 - 13:30	**Lunch Break**
AFTERNOON	

13:30 - 14:20	**Plenary Session 5** **INVERSE BAYESIAN PROBLEMS AS FILTERING MAPS** **Prof. Hermann G. Matthies |** Institute of Scientific Computing – Technische Universität Braunschweig | Germany
Session Chairs:	@Auditorium: @Room A: @Room B:
14:20 - 14:40	Presentation 2.13 **Paper 270** Matteo Riganti **Modelling of honeycomb composite sandwich panel with flax fiber skin** ISAE-SUPAERO - Institut Clément Ader – France **@Auditorium** Presentation 2.14 **Paper 261** Daniel de Bortoli **Fully coupled multi-scale finite element analysis of TRIP-assisted multi-phase alloys** INEGI Portugal **@Room A** Presentation 2.15 **Paper 204** Chaoqun Liu **New Vortex Identification Methods for Turbulence** University of Texas at Arlington USA **@Room B**
14:40 - 15:00	Presentation 2.16 Paper **236** Denis Düsseldorf **Construction of optimal basis functions in the Partition of Unity Method and their verification in complex simulations** University of Bonn Germany **@Auditorium** Presentation 2.17 **Paper 229** Matthias Birner **A Global-Local Zooming Technique** Fraunhofer Institut Germany **@Room A** Presentation 2.18 **Paper 243** Zhanli Liu **Designing phononic crystal with anticipated band structure through a deep learning based data-driven method** Tsinghua University China **@Room B**
15:00 - 15:20	Presentation 2.19 **Paper 233** Christine Espinosa **A fully coupled electromagnetic-thermal-transient mechanical simulation of the load suffered by aeronautical composite panels during lightning strikes** Institut Clément Ader France **@Auditorium** Presentation 2.20 **Paper 227** António M Couto Carneiro **Multiscale Moddeling of Self-Affine Rough Contact** INEGI Portugal **@Room A** Presentation 2.21 **Paper 277** Ashutosh Bhokare **Performance of drag models in CFD-DEM** Swansea University United Kingdom **@Room B**

15:20 - 15:40	Presentation 2.22 **Paper 268** Fazilay Abbes **Computational study of deformation mechanisms in hcp metal: Application to pure zinc** University of Reims Champagne Ardenne France **@Auditorium** Presentation 2.23 **Paper 263** Juan Manuel Calleja Vazquez **Multiscale stochastic simulations using a MFH model constructed from full-field SVE realizations** University of Liège Belgium **@Room A** Presentation 2.24 **Paper 228** Fangxin Fang **Multi-scale adaptive unstructured mesh predictive modelling for environmental problems** Imperial College United Kingdom **@Room B**
15:40-16h00	Coffee Break
16:00- 16:20	Presentation 2.25 **Paper 222** Sizeng You **Quantified Relationship between Properties of Fresh Self-compacting Concrete and Workability Test Performance** Swansea University United Kingdom **@Auditorium** Presentation 2.26 **Paper 278** Liang Yang PyEFEM **Massively parallel python based FEM framework for flow problems** Cranfield University United Kingdom **@Room A** Presentation 2.27 **Paper 219** Charles Henri Bruneau **Comparisons of direct numerical simulation and penalized models to compute the flow in a porous-fluid system** Université de Bordeaux | France **@Room B**
16:20 - 16:40	Presentation 2.28 **Paper 12** Bilen Emek Abali **Multiphysics Computation in Batteries Involving Electromagnetism and Thermomechanics** Technische Universitat Berlin | Germany **@Auditorium** Presentation 2.29 **Paper 202** Hyun Joon Chang **Examining the Mutation Effect of SLC26A4 STAS Domain By Observing the Communication Between Secondary Structures** Korea University | South Korea **@Room A** Presentation 2.30 **Paper 273** Srinivas Sriramula **Multi-scale Reliability Based Design Optimisation for Unidirectional FRP Composite Laminates** University of Aberdeen |United Kingdom **@Room B**
16:45	**DEPARTURE AND MINI BUS TOUR**
19:30	**ARRIVAL AT *CASA DA MUSICA* CONFERENCE DINNER**

CM4P ECCOMAS Thematic Conference

July 17th	
09:00-09:50	**Plenary Session 6:** **FRACTURE OF POLYMER COMPOSITE MATERIALS: SIMULATION ACROSS THE SCALES** **Prof. Pedro P. Camanho** | Faculty of Engineering – University of Porto
09:50- 10:00	**YOUNG RESEARCHERS AWARD CEREMONY**
10:00 -10:50	**Plenary Session 7** **MULTI-SCALE AND MULTI-PHYSICS CHALLENGES FOR FUTURE AIRCRAFT: A HIERARCHICAL APPROACH** **Paul Tucker** | Cambridge University United Kingdom
10:50-11:10	**COFFEE-BREAK**
Session Chairs:	@Auditorium: @Room A: @Room B:
11:10 -11:30	Presentation 3.1 **Paper 47** Jens-Dominik Müller_**Adjoint Based Optimisation of an Internal Cooling Channel U-Bend**_Queen Mary University of London United Kingdom_**@Auditorium** Presentation 3.2 **Paper 276** Jinsheng Wang_**Efficient structural reliability analysis based on polynomial chaos expansion and maximum entropy method**_Swansea University United Kingdom_**@Room A** Presentation 3.3 **Paper 46**_ Thiago Doca_ **Multi-uncertainty analysis of the indentation process of key engineering materials**_ University of Brasília – Brazil_**@Room B**

11:30-11:50	Presentation 3.4 **Paper 267**_ Shreyas Srivatsa_ **Micromechanical Modeling and Estimation of Elastic Properties of Pure MXene (Ti3C2Tx) Films**_ AGH University of Science and Technology Poland_**@Auditorium** Presentation 3.5 **Paper 255**_ Miguel V Carvalho_ **Computational Aspects on the Constitutive Modelling of Multiphase Alloys**_Faculty of Engineering of the University of Porto_Portugal_**@Room A** Presentation 3.6 **Paper 224**_ Abdelkhalak El Hami_ **Numerical modelling of the uncertainties in hip prosthesis material parameters** INSA Rouen France_**@Room B**
11:50 -12:10	Presentation 3.7 **Paper 247** Sule Ozturk_**A Turbulence Based Sensitivity Study on Drag Prediction of the NASA Common Research Model Aircraft**_Istanbul Technical University_Turkey**@Auditorium** Presentation 3.8 **Paper 259** Prattya Datta_ **PGD based domain decomposition method applied to parameterized seismic models**_Technical University of Barcelona_Spain_**@Room A** Presentation 3.9 **Paper 212**_ Victor Blanc_ **Dynamic Analysis of a Multi-Contact Problem Using Simplified Models to Study of the Influence of Clearances on Contact Forces**_ French Atomic and Alternatives Energies Commission_France_**@Room B**
12:10 -12:30	Presentation 3.10 **Paper 252** Farzad Shirazian_**A DFT study of single layer blue phosphorus and its implementation in a continuum model**_Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University | Germany**@Auditorium** Presentation 3.11 **Paper 210** Yizhi Shao_**Development of Multiscale Multi-physics Based Modelling and Simulations with the Application to Precision Machining of Aerofoil Structures**_Brunel University London | United Kigdom_**@Room A** Presentation 3.12 **Paper 271** Abdelkhalak El Hami_**Probablistic approach of a dynamic analysis of wind turbine on flexible foundation**_ INSA Rouen Normadie_France_**@Room B**

12:30-12:50	Presentation 3.13 **Paper 39**_ Nanda Gopala Kilingar_**Data driven computational analysis of open foam materials**_ University of Liége **@Auditorium** Presentation 3.14 **Paper 254**_Rui Coelho_ **Ductile failure analysis in metallic materials through computational homogenization_FEUP | Portugal @Room A** Presentation 3.15 **Paper 238** Abdelkhalak El Hami_**Metamodels for RBDO of wire bonding in microsystem packages**_ INSA Rouen Normadie_France_**@Room B**
12:50 -14:30	**Lunch Break**
14:30 -14:50	Presentation 3.16 **Paper 211**_Yanan Sun_**An Investigation of stepwise Crack Tip Advancement**_Swansea University_United Kigdom**@Auditorium** Presentation 3.17 **Paper 216** Jie Li_**The Refined Algrithm of Generalized Probability Density Evolution Equation Based on Reproducing Kernel Particle Method**_Tongji University Shanghai, China **@Room A** Presentation 3.18 **Paper 249**_ Ibrahim Cicek_**Optimization of Control Parameters for an Electrified Vertical Take-off Landing Vehicle Using the Integral Squared Method**_ Istanbul Technical University_Turkey **@Room B**
14:50-15:10	Presentation 3.19 **Paper 251** Alberto Moscatello_ **Scaling procedure for the design of a validation experiment on an accidental gas release** _ Politecnico di Torino Italy **@Auditorium** Presentation 3.20 TO BE CONFIRMED Presentation 3.21 TO BE CONFIRMED

Pore Water State in Heated Concrete—Comparing a Numerical Model to NMR Measurements

Christoph Pohl [1], Jörg F. Unger[1]

[1]Bundesanstalt für Materialforschung und -prüfung

christoph.pohl@bam.de

Spalling of concrete structures is a serious issue for their safety. A better understanding of the pore water distribution and state during a fire is a prerequisite for numerical approaches to such problems.

Temperature-driven water transport in concrete consists of multiple phenomena, such as convection, diffusion, adsorption and dehydration. Distinguishing the different influences experimentally is difficult because typically they cannot be disentangled.

A common experimental setup approximates a one-dimensional flow, and places temperature and pressure gauges along the propagation direction [1]. For direct information about the water content inside a sample, methods such as NMR or neuron radiography are necessary.

A multiphase model for the flow in porous media based on [2] is presented, with dehydration and changes in the pore size distribution taken into consideration. NMR measurements for temperature-driven flow have been performed. The numerical and experimental results are compared for water transport at temperatures below the critical point. Since both the finite-element model and the experiment allow the distinction between adsorbed, capillary and bulk water, a more fine-grained view of the pore water state is obtained.

[1] P. Kalifa, F.-D. Menneteau and D. Quenard, "Spalling and pore pressure in HPC at high temperatures," *Cement and Concrete Research,* vol. 30, pp. 1915-1927, 2000.

[2] D. Gawin, F. Pesavento and B. A. Schrefler, "What physical phenomena can be neglected when modelling concrete at high temperature? A comparative study. Part 1: Physical phenomena and mathematical model," *International Journal of Solids and Structures,* vol. 48, p. 1927–1944, Jun 2011.

Computationally efficient homogenization for modeling of nonlinear functionally graded materials

Witold Ogierman [1]

[1]Silesian University of Technology, Gliwice, Poland

witold.ogierman@polsl.pl

Advanced composite materials such as functionally graded particle reinforced composites can provide unique properties due to spatially varied microstructural features. In this case prescribed properties of structural elements can be achieved for example by controlling the spatial distribution of the reinforcement. Design of such materials and prediction of their effective properties can be performed by using advanced computational methods. The present investigation is devoted to development of computationally efficient homogenization procedure for modeling of particle reinforced functionally graded materials (FGM) that exhibit elastic-plastic properties. At the macroscopic level the FGM can be regarded as material consisting of multiple layers with different volume fraction of the reinforcement [1]. The material properties of the layers can be determined in terms of microstructural features like the reinforcement volume fraction, shape etc. by using the homogenization procedure. One of the most widely used and versatile method of homogenization is based on finite element (FE) analysis of representative volume element (RVE). The FE based homogenization can be applied in modelling of nonlinear constitutive behavior and microstructures of complex geometry however in such cases it typically requires time consuming computations [2]. Moreover generation of different RVEs for different layers and usage of strongly coupled multi-scale FE^2 framework could lead to prohibitive time of computations. The other way is to use the mean field homogenization approaches among which the most popular is the Mori-Tanaka (M-T) method which provides good predictive capabilities and low computational cost. On the other hand the M-T method is limited to the case of the ellipsoidal shape of the reinforcement only for which the fundamental Eshelby's solution is valid [3]. In addition, methods of isotropic approximation of tangent stiffness tensor are required in order to achieve a reasonable accuracy for elastic-plastic materials. Nevertheless, these limitations can be overcome by using numerical solution of the single

inclusion problem instead of using Eshelby's fundamental solution [4, 5]. Generally, such a hybrid M-T/FE method is more versatile than analytical M-T method and provide more time-efficient solution than pure FE method. The present study is devoted to application of novel simplified homogenization method for modeling of elastic-plastic FGMs based on the hybrid M-T/FE. The idea is to obtain the nonlinear mean field relation between the macroscopic strain and the strain in the reinforcement by solving the Eshelby's problem numerically only once and then approximate the properties of layers containing different volume fractions of the reinforcement analytically. This approach may lead to achieve very time-efficient solution while simultaneously providing high accuracy.

The presentation will cover mainly: details of the numerical procedures connected with the novel homogenization method, discussion on accuracy of proposed method both in linear-elastic and nonlinear regime, comparison of the obtained results with the results of homogenization based on finite element (FE) analysis of the representative volume element (RVE) containing complex geometry, examples illustrating a potential and effectiveness of the proposed approach.

Acknowledgement

The research for this paper was financially supported by the National Science Centre, Poland (Grant No. UMO-2016/21/N/ST8/01119) and the Silesian University of Technology (Grant No. 10/040/RGJ19/0081).

References

1. Schmauder, S., Weber, U. Modelling of functionally graded materials by numerical homogenization, *Archive of Applied Mechanics*, 71(2), 182-192, 2001

2. Ogierman, W., Kokot, G. Generation of representative volume elements of heterogeneous materials with distributed orientations of inclusions. *Composite Structures*, 201, 636–646, 2018.

3. Eshelby, J. D. The determination of the elastic field of an ellipsoidal inclusion, and related problems. *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, 241(1226), 376–396, 1957.

4. Brassart, L., Doghri, I., Delannay, L. Homogenization of elasto-plastic composites coupled with a nonlinear finite element analysis of the equivalent inclusion problem. *International Journal of Solids and Structures*, 47(5), 716–729, 2010.

5. Ogierman, W. Hybrid Mori-Tanaka/Finite Element Method in Homogenization of Composite Materials with Various Reinforcement Shape and Orientation, *International Journal for Multiscale Computational Engineering* (In Press), 2019.

Multiphysics Computation in Batteries Involving Electromagnetism and Thermomechanics

Bilen Emek Abali [1]

[1]Technische Universität Berlin, Institute of Mechanics, Einsteinufer 5, 10587 Berlin, Germany

bilenemek@abali.org

An electrochemical cell like a Li-ion battery has to be modeled by involving multiphysics phenomena called and studied separately. Electromagnetism is governed by Maxwell equations; thermomechanics is given by balance equations, all these equations are incompatible with each other making a derivation of the unique and consistent theory very challenging. In the case of electro-thermo-mechanical systems, we established the derivation of all necessary equations by using theoretical thermodynamics[1] and their accurate computation[2] by using a monolithic solution technique[3] based on open-source packages developed and known under the FEniCS project.[4]

This talk is on the extension of the theoretical framework for incorporating diffusion as a result of balance equations for every constituent---this approach is called the mixture theory in continuum mechanics. As a system alike Li-ion battery consolidates all possible physical phenomena in a continuum body, we need to solve coupled and nonlinear field equations in a monolithic approach. Especially in electromagnetism, there are various methods to circumvent emerging numerical problems. Hence, a strong emphasis will be put on the computation of electromagnetic fields in a robust algorithm.

[1] Abali, B. E., & Reich, F. A. (2017). Thermodynamically consistent derivation and computation of electro-thermo-mechanical systems for solid bodies. Computer Methods in Applied Mechanics and Engineering, 319, 567-595.
[2] Abali, B. E., & Reich, F. A. (2018). Verification of deforming polarized structure computation by using a closed-form solution. Continuum Mechanics and Thermodynamics, 1-16.
[3] Abali, B. E. (2017). Computational Reality: Solving Nonlinear and Coupled Problems in Continuum Mechanics. Springer Nature, Singapore.
[4] https://fenicsproject.org/

Presenting Author, Second Author, Third Author

On modeling interfaces in composite with multi-physic coupling

Michele Serpilli [1], Raffaella Rizzoni [2], Serge Dumont [3], Frédéric Lebon[4]

[1]Università Politecnica delle Marche, Ancona, Italy

m.serpilli@univpm.it

[2]Università di Ferrara, Ferrara, Italy

raffaella.rizzoni@unife.it

[3]Université de Nîmes, Nîmes, France

serge.dumont@unimes.fr

[4]Aix-Marseille Univ, CNRS, Centrale Marseille, France

lebon@lma.cnrs-mrs.fr

In the last decades, the interest in bonded structures, obtained by assembling different parts made of possibly different materials to compose a unique structure, is strongly increased. The advantage of such composites is that their mechanical performances and properties are designed to be superior to those of the constituent materials acting independently. Nowadays, composites have been more frequently used in civil, naval, aeronautical and mechanical engineering, in general. The bond among the various parts of the composite may generally be imperfect and discontinuities in physical fields can arise, significantly changing the mechanical and physical properties of the material. Hence, a correct theoretical modeling of the imperfect bonding plays an important role in engineering design.

In the present work we focus our attention to a specific type of composite, constituted by two media, called the adherents, bonded together with a thin interphase layer, called the adhesive. We assume that the composite constituents are made of different multi-physic materials with highly contrasted constitutive properties. The study considers a generic multi-physic coupling in a very general framework and can be adapted to well-known multi-physic behaviors, such as piezoelectricity, thermo-elasticity, magneto-electro-thermo-elasticity, as well as to multifield microstructural theories, such as micropolar and microstretch elasticity. The analysis has been carried out by means of asymptotic expansions method. The use of this technique spans from the justification of classical theories of thin structures [1] to the rigorous derivation of simplified models for complex assemblies, presenting thin interphases, in the field of linear elasticity [2] as well as in piezoelectricity, taking into account thermal, magnetic and other physical interactions [3,4]. The asymptotic methods allow to replace the adhesive layer with a two-dimensional surface, the so-called imperfect interface, with non-classical transmission conditions between the two adherents.

By defining a small parameter ε, associated with the thickness and constitutive properties of the middle layer, we perform an asymptotic analysis. We assume that the thickness depends linearly on ε, while the multi-physic stiffness ratios between the adherents and the adhesive depends on ε^p. We identify three critical exponents p, corresponding to different imperfect interface models: p=1, the *soft* (also called *lowly-conducting*) multi-physic interface model, for which we rescale the constitutive coefficients of the intermediate layer with ε; p=0, the *hard* (also called *moderately-conducting*) multi-physic interface model, for which the rigidities of the constituent materials have the same order of magnitude; p=-1, the *rigid* (also called *highly-conducting*) multi-physic interface model, for which we choose 1/ε as rescaling. Following the approach by [2], we derive the limit transmission problem at order zero. Moreover, taking into account higher order terms of the asymptotic expansion, namely the first corrector terms, we give a more precise approximation of the actual mechanical behavior of the interface. Finally, a general multi-physic interface model has been developed, including the three aforementioned limit behaviors, and numerically tested through the finite element method. In particular, in the framework of piezoelectricity, we compare the results obtained by modeling the adhesive as an interphase, having a thin finite thickness, with the results obtained with the general multi-physic interface model.

References.

[1] Ciarlet PG Mathematical Elasticity, vol. II: Theory of Plates. North-Holland, Amsterdam, 1997.
[2] Rizzoni R, Dumont S, Lebon F, Sacco E (2014) Higher order models for soft and hard elastic interfaces. Int. J. Solids Struct. 51(23-24): 4137-4148.
[3] Serpilli M (2015) Mathematical modeling of weak and strong piezoelectric interfaces, J. Elasticity 121(2): 235-254.
[4] Serpilli M (2017) Asymptotic interface models in magneto-electro-thermo-elastic composites. Meccanica 52(6): 1407-1424.

Sub-Modeling Approach to Investigate the Cracking Behavior of Reinforced Concrete Structures Considering Polymorphic Uncertainty

Katharina Kremer [1] , Philipp Edler [1], Steffen Freitag [2], Günther Meschke [1]

[1] Ruhr University Bochum, Germany
{katharina.kremer, philipp.edler, guenther.meschke}@rub.de

[2] Ruhr University Bochum, Germany
steffen.freitag@sd.rub.de

The cracking behavior of reinforced concrete (RC) structures is influenced, beyond temperature and loading, by the reinforcement design and the bond characteristics between the steel reinforcement and the concrete. In this contribution, a RC two-span beam subjected to its self-weight and a traffic load, is investigated regarding the crack pattern and the evaluation of crack widths, considering uncertainties of material data. A sub-modeling approach is used for investigating only highly stressed parts of the structure with a detailed model taking the boundary conditions from a coarse structural model into account to reduce the computation time. In a first step, the RC beam is analyzed with a continuum damage model to identify the critical sections ("hot spots"), where cracks are expected to appear. In the next step, the identified hot spots are analyzed with a more refined model enabling a discrete representation of cracks via cohesive interface elements [1]. In both models, the reinforcement is considered by means of a discretization independent embedded rebar model, where frictional contact between steel reinforcement and concrete is taken into account to consider the tension stiffening [2].

The main factors, which influence the cracking behavior (onset of cracking and crack width) of RC structures, are the tensile strength, the Young's modulus and the concrete-steel bond characteristics. These parameters are considered as uncertain parameters within the simulation. In general, aleatoric uncertain parameters, which are concerned with randomness, are quantified by stochastic distributions and epistemic uncertain parameters, which deal with lack of knowledge, are quantified by intervals or fuzzy numbers. In this contribution, the Young's modulus, which is assumed as fully correlated to the concrete strength according to fib Model Code [3], is considered as a stochastic parameter, which is lognormal distributed. The traffic load is also described by a stochastic parameter, using a Gaussian distribution. For investigating the influence of

imprecise rebar bond behavior to the cracking behavior, the bond strength is considered as an epistemic uncertain parameter. In the fib Model Code [3] the maximal bond strength τ_{max} is proposed as a function of the compressive strength. This value is taken as a reference value, to quantify the interval bounds for the bond strength.

In a first investigation [4] the influence of the polymorphic uncertain parameters was already investigated for a 2D Finite Element (FE) simulation with chosen reinforcement of five rebars with a diameter of 20 mm for the lower and upper reinforcement layers based on a classical reinforcement design. It was found, that for a fixed Young's modulus of concrete the lower and upper bound of the bond strength has almost no influence to the load-displacement curve for the full structural model, but the comparison of the crack pattern of the sub-models for the lower and upper bound of the bond strength shows significant difference in crack widths and crack patterns, which, in turn, affects the durability of the structure. In this contribution, results from a 3D simulation of the RC beam using polymorphic uncertain parameters are presented. Here, the focus will be on the influence of the reinforcement design (smaller vs. larger diameters with same area of reinforcement), considering uncertain bond strength, on the distribution of the crack pattern and crack widths, respectively.

References

[1] Zhan, Y.; Meschke, G.: Multilevel computational model for failure analysis of steel-fiber-reinforced concrete structures. Journal of Engineering Mechanics (ASCE), 142, 2016, pp. 1-14.

[2] Gall, V. E.; Butt, S.; Neu, G.; Meschke: An embedded rebar model for computational analysis of reinforced concrete structures with applications to longitudinal joints in precast tunnel lining segments. In: G. Meschke, G.; Pichler, B.; Rots, J. G. (Eds.), Computational Modelling of Concrete Structures (EURO-C 2018), CRC press, 2018, pp. 705-714.

[3] International Federation for Structural Concrete CEB-FIP Model Code 1990 (Design Code), Thom, 1993.

[4] Kremer, K.; Edler, P.; Miska, N.; Leichsenring, F.; Balzani, D.; Freitag, S.; Graf, W.; Kaliske, M.; Meschke, G.: Modeling of structures with polymorphic uncertainties at different length scales. Surveys for Applied Mathematics and Mechanics (GAMM-Mitteilungen), 2019, accepted.

A computational multi-physics model to predict The chemo-mechanical degradation of historical oil paintings

Emanuela Bosco [1], Gijs J.A.M. Eumelen [1], Akke S.J. Suiker [1]

[1]Eindhoven University of Technology, The Netherlands

e.bosco@tue.nl

A common, yet critical degradation mechanism in historical oil paintings is related to the formation and growth of metal soap crystals. Historical oil paintings typically consist of layers of a drying oil binding medium that contains metal-based pigment particles. The chemical reaction between the metal ions present in the pigments and the saturated fatty acids released by oil binder results in the formation of metal soaps, which can crystallize and grow into large protrusions [1]. This originates mechanical strains in the system, deforming paint layers and ultimately leading to cracking, flaking and delamination of the paint. This work presents a computational multi-physics framework to predict the degradation of historical oil paintings induced by metal soap formation and growth. The chemical processes are described through a diffusion-reaction model [2] formulated by taking the saturated fatty acids as the reference diffusing species. The reaction term allows to represent the formation and growth of a metal soap crystal. A chemically-induced growth strain introduces the coupling between the chemical and the mechanical models, by quantifying the effect of metal soap growth on the stress field generated in the paint system. Further, the change in mechanical properties associated to the formation of crystalline metal soap is described through a rule of mixtures based on the volume fractions of formed metal soap and the original oil binder material. The proposed model is implemented within a finite element setting, combined with a discrete crack approach, for which cohesive interface elements are placed between all continuum elements discretizing the paint layer geometry. The nucleation and propagation of cracks is prescribed according the interface damage model proposed in [3]. Furthermore, across crack faces, the constitutive relation between the flux and the concentration of saturated fatty acid is given as a function of mechanical damage. The numerical update procedure of the coupled chemo-mechanical processes is performed by using a staggered scheme. A set of numerical simulations illustrates the capability of the model to predict metal soap

crystallization and growth and the fracture induced in the paint. The study finally illustrates the influence of different chemical and mechanical parameters (elastic stiffness mismatch between the paint and the metal soap crystal, chemical growth strain and reaction rate) on the chemo-mechanical degradation of the paint layer.

References

[1] J. J. Hermans, K. Keune, A. van Loon, P. D. Iedema, An infrared spectroscopic study of the nature of zinc carboxylates in oil paintings, Journal of Analytical Atomic Spectrometry 30 (7) (2015) 1600-1608.

[2] T. S. Hille, S. Turteltaub, A. S. J. Suiker, Oxide growth and damage evolution in thermal barrier coatings, Engineering Fracture Mechanics 78 (10) (2011) 2139-2152.

[3] M. V. Cid Alfaro, A. S. J. Suiker, R. de Borst, J. J. C. Remmers, Analysis of fracture and delamination in laminates using 3D numerical modelling, Engineering Fracture Mechanics 76 (6) (2009) 761-780.

A coupled chemo-mechanical model for biogenic Sulfide corrosion in concrete sewer pipes

Emanuela Bosco [1], Frits A.M. Rooyackers[1], Akke S.J. Suiker [1], Francois H.L.R. Clemens[2,3]

[1]Eindhoven University of Technology, The Netherlands

[2]Delft University of Technology, The Netherlands

[3]Deltares,The Netherlands

e.bosco@tue.nl

Durability of concrete is a relevant issue in the structural design of sewer systems, which largely impacts the maintenance and rehabilitation costs associated to the sewerage infrastructure. In this context, chemical attacks by sulfates, and in particular biogenic sulfide corrosion, are primary causes of concrete degradation. Biogenic sulfide corrosion is caused by Thio-oxidans bacteria, which may grow on the surface of concrete above the wastewater level in relative acidic environments. These bacteria are able to oxidize sulfur compounds into sulfuric acid that may diffuse into the concrete pipe, reacting with calcium hydroxide to form gypsum and ettringite [1]. These newly formed compounds have only limited structural properties. Additionally, they occupy a larger volume than the original material, introducing an expansive strain that can result in the cracking of concrete and in the loss of aggregates. Conversely, cracking phenomena influence the diffusivity of the system, thus further promoting the ingress of sulfuric acid and accelerating concrete degradation.

This contribution precisely proposes a coupled chemo-mechanical model to predict biochemical degradation of concrete sewer pipes. While some recent works in the literature deal with the numerical simulation of the biochemical degradation process by mainly considering ettringite formation [2, 3], this study focuses on the process of gypsum formation. The chemical model accounts for several (diffusion-) reaction equations, coupled by their reaction terms. A chemical strain, defined as a function of gypsum concentration, allows to represent the expansive nature of gypsum. Further, the governing constitutive equations are formulated as a function of chemical and mechanical damage parameters, which account for the effects of chemical and mechanical degradation. The

model is implemented within the finite element framework. A series of numerical simulations is performed on a sewer pipe geometry, providing the concentration evolutions of the relevant chemical species in the system and demonstrating the capability of the model to adequately estimate the development of damage.

References

[1] Davis, J., Nica, D., Shields, K., & Roberts, D. (1998). Analysis of concrete from corroded sewer pipe. International Biodeterioration & Biodegradation, 42, 75–84.

[2] Idiart, A., Lopez, C., & Carol, I. (2010). Chemo-mechanical analysis of concrete cracking and degradation due to external sulfate attack: A meso-scale model. Cement and Concrete Composites, 33, 411–423.

[3] Cefis, N., & Comi, C. (2017). Chemo-mechanical modelling of the external sulfate attack in concrete. Cement and Concrete Research, 93, 57–70.

Degradation of Lithium-Ion Batteries in Aerospace

Linda J. Bolay[1,2], Birger Horstmann[1,2], Omar S. Mendoza-Hernandez[4], Yoshitsugu Sone[4,5], Arnulf Latz[1,2,3]

[1] Institute of Engineering Thermodynamics, German Aerospace Center, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany

[2] Helmholtz Institute Ulm for Electrochemical Energy Storage, Helmholtzstrasse 11, 89081 Ulm, Germany

[3] Institute of Electrochemistry, University of Ulm, Helmholtzstrasse 11, 89081 Ulm, Germany

[4] Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency, 3-1-1 Yoshinodai, Chuo-ku, Sagamihara, Kanagawa, 252-5210 Japan

[5] The Graduate University of Advanced Studies (SOKENDAI), 3-1-1 Yoshinodai, Chuo-ku, Sagamihara, Kanagawa, 252-5210 Japan

linda.bolay@dlr.de

Lithium-ion batteries are the technology of choice for a broad range of applications due to their performance and long-term stability. The performance and durability of lithium-ion batteries is heavily impacted by various degradation mechanisms. These include the growth of the solid-electrolyte interphase (SEI) and the deposition of metallic lithium on the surface of the negative electrode, referred to as lithium plating. Long-term SEI growth is the biggest contributor to capacity fade in lithium-ion batteries. Lithium plating, which occurs in low temperature or high current charging, can result in capacity fade or even thermal runaway.

In our group we develop multiphysical models and perform simulations for various types of batteries. In order to describe the internal processes of Li-ion batteries, we derive thermodynamic consistent transport theories [1]. Based on these, our group has developed models for long-term SEI growth [2,3] and for lithium plating in 3D electrode microstructures [4].

Such models predict battery performance over short time scales during single charging and discharging as well as battery degradation over long time scales during continued cycling.

Finally, we want to understand the processes taking place in Li-ion batteries and observe them during battery operation. Here, we discuss perfomance and lifetime for the batteries of in-orbit satellite REIMEI [5]. To this end, we parameterize our model by comparing the electrochemical simulations to various experimental and in-flight data. By incorporating our new model for continued growth of the SEI [2], we simulate degradation in micro-structured electrodes in one and three dimensions. We are the first to understand experimentally observed inhomogeneities in the SEIs thickness throughout the negative electrode. Furthermore, our degradation model applies to battery storage as well as to battery cycling. We will further discuss lithium plating and perform state estimation of the REIMEI battery to predict its state-of-health in earth orbit.

References:

[1] A. Latz, J. Zausch, Beilstein Journal of Nanotechnology 6 (2015) 987, doi:10.3762/bjnano.6.102.

[2] F. Single, A. Latz, B. Horstmann, ChemSusChem 11(12) (2018) 1950-1955, doi: 10.1149/2.0121711jes.

[3] F. Single, B. Horstmann, A. Latz, Journal of The Electrochemical Society 164(11) (2017) E3132-E3145. doi:10.1149/2.0121711jes.

[4] S. Hein, A. Latz, Electrochimica Acta 201 (2016) 354-365, doi: 10.1016/j.electacta.2016.01.220.

[5] M. Uno, K. Ogawa, Y. Takeda, Y. Sone, K. Tanaka, M. Mita, H. Saito, Journal of Power Sources 196(20) (2011) 8755-8763, doi:10.1016/j.jpowsour.2011.06.051.

Reduced-order Modelling Scheme for Problems with Fully Resolved Microstructures Generated by Generalized Periodic Unit Cells

Martin Doškář [1], Jan Novák [1], and Jan Zeman [1]

[1]Czech Technical University in Prague

martin.doskar@fsv.cvut.cz

Microstructural details influence the performance of products especially when it comes to localizing phenomena and problems with low separation of microstructural and macroscopic scales. However, hardly ever the actual microstructural composition within a macroscopic product is a-priori known, thus a statistical quantification of product responses under varying microstructural realizations is desired. This may require (i) procedures for generating random yet statistically coherent realizations of a given microstructure and (ii) efficient numerical schemes for related analyses.

Addressing the first requirement, we have proposed a representation of material microstructures built on the formalism of Wang tiles (Novák et al., 2012). Our approach delivers a compromise between the (Statistically Equivalent) Periodic Unit Cell characterization of material microstructures and an approach in which stochastic microstructural realizations are generated each time anew (e.g. using costly optimization approaches). With only a handful of small microstructural cells – Wang tiles – with predefined mutual compatibility arbitrarily large, stochastic microstructural samples can be generating following a simple stochastic assembly algorithm. In our previous works, only the geometrical part of the tile-based representation has been utilised, e.g. (Doškář et al., 2018). However, given the repeating occurrence of individual tiles in the assembled microstructural realizations, the tile-based representation holds promise also for addressing the second requirement.

In this contribution, we present a numerical scheme that combines the eXtended Finite Element Method (XFEM) and Reduced Order Modelling (ROM) to accelerate numerical analyses of macroscopic problems whose microstructural geometry was generated by means of Wang tiles. The scheme comprises two ingredients. First, inspired by numerical homogenization, we extract characteristic fluctuation responses of the microstructure at the level of the compressed tile representation. Second, we combine

a coarse finite element discretization (unaware of the underlying microstructure) of a macroscopic problem and the assembled characteristic fluctuations using an XFEM ansatz. While the macroscopic discretization captures the global character of a macroscopic response, the XFEM ansatz serves as an interpolation between assembled fluctuation modes, which were derived without any knowledge of the shape or loading of the macroscopic problem. The scheme thus differs from standard ROM approaches as we don't sample a parametric space and extract response of the macroscopic problem; in this sense, it resembles more the XFEM formulations with dictionary solutions, e.g. (Strouboulis et al., 2003). On the other hand, we adopt the ROM perspective in implementation due to its straightforward way of posing Dirichlet boundary conditions and potential for additional acceleration by means of hyper-reduction methods.

Acknowledgement

This work was partially funded by the Ministry of Industry and Trade of the Czech Republic through the project No. FV10202. In addition, MD and JN acknowledge the financial support through OP VVV projects International Mobility of Researchers Nos. CZ.02.2.69/0.0/0.0/16_027/0008465 and CZ.02.2.69/0.0/0.0/17_050/0008025.

References

Doškář, M., Zeman, J., Jarušková, D., Novák, J., 2018. Wang tiling aided statistical determination of the Representative Volume Element size of random heterogeneous materials. European Journal of Mechanics - A/Solids 70, 280–295. https://doi.org/10.1016/j.euromechsol.2017.12.002

Novák, J., Kučerová, A., Zeman, J., 2012. Compressing random microstructures via stochastic Wang tilings. Physical Review E 86, 040104(R). https://doi.org/10.1103/PhysRevE.86.040104

Strouboulis, T., Zhang, L., Babuška, I., 2003. Generalized finite element method using mesh-based handbooks: application to problems in domains with many voids. Computer Methods in Applied Mechanics and Engineering 192, 3109–3161. https://doi.org/10.1016/S0045-7825(03)00347-5

Fragment size characterization for granular flow in highly damaged ceramics

Lori Graham-Brady [1], Amartya Bhattacharjee [1]

[1]Johns Hopkins University

lori@jhu.edu

Granular mechanics has been studied extensively, particularly in the field of geomechanics. However, the onset of granular mechanics and flow characteristics in a dense comminuted brittle material is still not well understood. We know that the initial grain size distribution plays an important role in determining granular flow characteristics. Under brittle dynamic compression loading, as often observed in impact experiments, wing crack- growth from pre-existing defects, subsequent crack interactions and coalescence mechanisms lead to fragmentation and granular flow in highly damaged regions. This talk focusses on determining an approximate initial fragment size distribution for granular flow and can be used in general, to obtain fragment size statistics from crack size statistics. Crack populations have been numerically simulated from a known distribution on effective length and orientation of cracks, and later stage coalescence has been accounted for by using a threshold distance around a crack tip. Fragment statistics, like size and shape distribution have been obtained by using a connected region-based algorithm. The same approach has been extrapolated in three dimensions, but here the cracks have been simulated as elliptical cracks with a thick ring around the edges. The ring size accounts for the threshold coalescence distance, and is obtained using crack-bridge strength calculations. Fragments, as before, are obtained as connected regions, and then allowed to dilate till they fill up the space. Preliminary investigation hints at a power law based distribution for fragment sizes. Although the particular problem has been set to obtain fragment size statistics from prior information about cracks, they can also be used to obtain a general fragmentation criterion.

Development of a modified Voronoi's tesselation algorithm for the determination of the effective properties of cork-based composites

Marco Delucia [1], Anita Catapano [2], Marco Montemurro [1], Jérôme Pailhès [1]

[1] Laboratoire I2M, CNRS UMR 5295, Arts et Métiers ParisTech, 33400 Talence (France)

marco.delucia@ensam.eu, marco.montemurro@ensam.eu and jerome.pailhes@ensam.eu

[2] Laboratoire I2M, CNRS UMR 5295, Bordeaux INP, Université de Bordeaux, 33400 Talence (France)

anita.catapano@bordeaux-inp.fr

Cork is a natural, recyclable and biodegradable industrially useful material with remarkable properties as lightness, excellent thermal and sound insulating properties mainly due to its honeycomb-like microstructure. Cork is extracted periodically, in a sustainable manner, from the outer bark of *Quercus Suber L.* and, depending on the type of final product, it can be exploited directly in its natural form or it can be used as cork-based agglomerate or composite [1] wherein the cork granules are mixed with a polymeric binder.

The mesostructure of cork agglomerates is characterized by randomly distributed polygonal particles which, combined with the complex microstructure of the cork, leads to complex stress/strain distributions and damage mechanisms. Omitting the effects of the honeycomb microstructure of the cork, macroscopic thermal and elastic behaviour of cork-based agglomerates depends upon different parameters defining the mesoscopic representative volume element (RVE) of the agglomerate: spatial orientation and shape of the grains, material properties of matrix and cork (including anisotropy of cork) as well as their volume fraction, percentage of voids and the matrix/grain interface properties [2,3].

The aim of the present work is to propose a general multi-scale numerical homogenisation procedure capable of determining the effective thermal and elastic properties of cork-based agglomerates. The fundamental aspect on which the proposed work is focused consists in generating a realistic mesostructural geometry of the cork-based composite. More precisely, a 2D as well a 3D parametric computational model based on a modified Voronoi’s tessellation algorithm has been developed and the strain

energy homogenisation technique for heterogeneous media [4] has been used for determining the effective properties of the agglomerate at the macroscale level. In this new algorithm for mesostructure generation, several aspects of fundamental importance have been taken into account:

- the polygonal shape of cork particles that show sharp angles, convexities and concavities;
- the transversely isotropic mechanical behavior of cork, whose material frame is randomly oriented within the mesostructured;
- the random geometrical orientation of cork particles;
- the high variability of cork mechanical properties;
- the variability of porosity distribution.

All these aspects have been considered in the development of the algorithm which has been coded in Python environment.

The 2D and 3D artificial mesostructures have been utilized to perform the strain-energy based homogenisation of elastic and thermal properties of different cork-based composites and the Monte Carlo method has been used to take into account the variability of the parameters at the mesoscale on the equivalent thermo-elastic behaviour at the macroscopic scale.

Numerical results have been compared firstly to the numerical ones obtained on mesostructures achieved by means of the digital image correlation (DIC) technique and then to the experimental ones in order to show the effectiveness of the proposed procedure.

[1] H. Pereira, *Cork: Biology, Production and Uses*, 2007.

[2] P. T. Santos, S. Pinto, P. A.A.P. Marques, A. B. Pereira, and R. J. Alves de Sousa. *Agglomerated cork: A way to tailor its mechanical properties*. Composite Structures, 178:277-287, 2017.

[3] P. T. Santos, J. S. Amaral, V. A. F. Costa, and V. S. Amaral. *Thermal Conductivity of Agglomerate Cork*. In Materials Research Proceedings, Volume 3, 1-10, 2017.

[4] E. J. Barbero. *Finite element analysis of composite materials using ansys*. 2013.

Data driven computational analysis of open foam materials

Nanda Gopala Kilingar[1], Ludovic Noels[1], Thierry J. Massart[2]

[1]Université de Liège (ULiège)

ngkilingar@uliege.be

[2]Université Libre de Bruxelles (ULB)

An automated approach, that relies on the use of distance and level set functions as explained in [1], has been described in [2] to build computationally Representative Volume Elements (RVE) of open foam materials, enabling the study of the effects of the microstructural features on the macroscopic behavior. These models have been compared with real foam samples from existing literature to verify statistically the morphological properties like face-to-cell ratio, edge-to-face ratio and strut length distribution along with the variations in the strut morphology like the shape of cross-sections of the struts and their variation along the axis of the struts. The responses obtained from a uniaxial compression test of the sample RVEs have been validated against the experimental observations and the results have showed close similarity with respect to the variations in the foam density. This approach enables us to generate multiple Stochastic volume elements (SVE) and get their material response in a short period of time.

In [3], the authors have taken inspiration from artificial neural network concepts and used linear elastic RVE data to train a material network to describe complex material

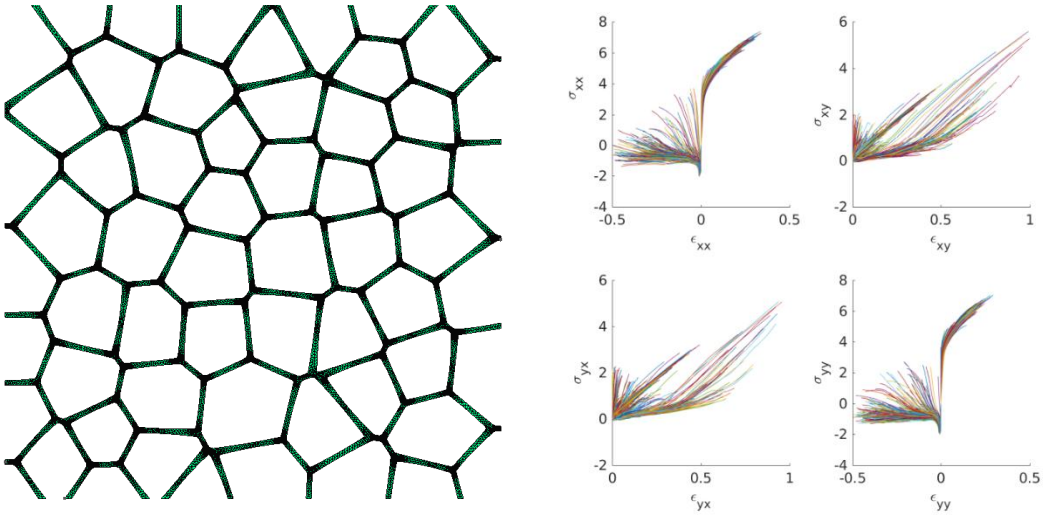


Figure 1 A 2D RVE of an open foam and its response to various deformation loads

behavior. They have also validated the extrapolations of the trained network to a wide range of problems, including non-linear history-dependent plasticity and finite-strain hyper-elasticity under large deformations.

In the current work, the goal is to utilize the material responses obtained from the SVEs as the prespecified material data set (Figure 1) and investigate the performance of various data-driven solvers on these data sets in order to eliminate the experimental testing altogether with the knowledge that the material response is in close agreement to that of the RVEs.

References

[1] B. Sonon, B. Francois and T. J. Massart, "An advanced approach for the generation of complex cellular representative volume elements using distance fields and level sets," *Computational Mechanics*, 2015.

[2] N. G. Kilingar, K. Ehab Moustaa Kamel, B. Sonon, T. J. Massart and L. Noels, "Computational generation of open-foam representative volume elements with morphological control using distance fields," *Under review*.

[3] Z. Liu, C. T. Wu and M. Koishi, "A Deep Material Network for Multiscale Topology Learning and Accelerated Nonlinear Modeling of Heterogeneous Materials," *Computer methods in applied mechanics and engineering*, 2018.

Simulation Model for Single unit Warpage of Shadow moire in Flip-Chip Process

Wan-Chun Chuang [1,2*], Wei-Long Chen [1]

[1] Department of Mechanical and Electro-Mechanical Engineering, National Sun Yat-sen University, Kaohsiung, Taiwan, R.O.C.

[2] Department of Sports Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan, R.O.C.

wcchuang@mail.nsysu.edu.tw

Background

The demand for lightweight and high functionality devices is always in the development of the smaller and lighter package technology so that Flip-Chip and Wafer-Level package technology develop. In 2018 S. J. Oon [1] mentioned that because of the CTE(Coefficient of Thermal Expansion) mismatch of the materials, thus, the package structure will occur warpage in a heating process such as Shadow moire. Worst of all, warpage will result in low yields on the production line.

Research Methods

The research process comprised two steps: 1) setup simulation model and boundary condition, 2) setup material parameter. (1)Simulation model and boundary conditions: COMSOL Multiphysics simulation software was used to establish single unit simulation model. The geometry of model as follows: PKG was 7*7*0.45 mm^3, die was 6.3*6.34*0.23 mm^3, bump pitch was 0.19 mm, and solder ball diameter was 0.25 mm. The boundary condition was set as scroll between the end of the single unit model and the ground. Besides, the temperature was 25°C →260°C→25°C and process time was 1100s for shadow moire measurement. (2) Material parameter: Tables 1 list the material parameters settings of the bump, silicon and substrate. All the materials were isotropic in this study. However, the properties of the compound were easily affected by temperature. Therefore, the compound was measured with DMA(Dynamic Mechanical Analysis) and TMA(Thermomechanical Analysis) at different temperatures, Fig. 1 illustrates the Young's modulus and CTE of compound.

Tables 1: Material parameters of the bump, silicon and substrate

	Bump SAC405	**Silicon<100> (Die)**	**Substrate**
Young's modulus (GPa)	53	131	26 (25°C),15 (260°C)
Poisson's ratio	0.40805	0.27	0.2
Density (kg/m^3)	7445.45	2330	1938

CTE(ppm/°C)	20	2.8	15 (25°C),6 (260°C)

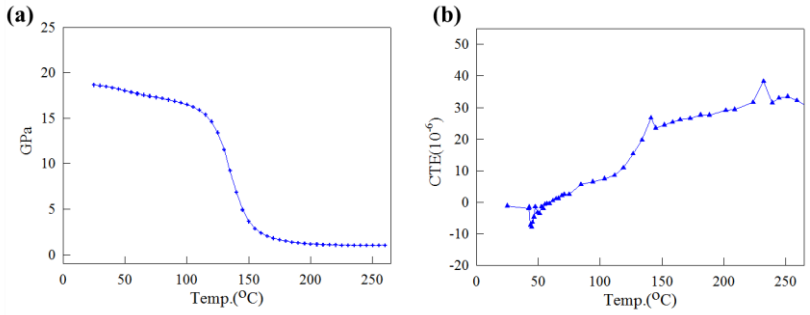


Fig. 1: Material parameters of compound at different temperatures: (a) Young's modulus; (b) CTE。

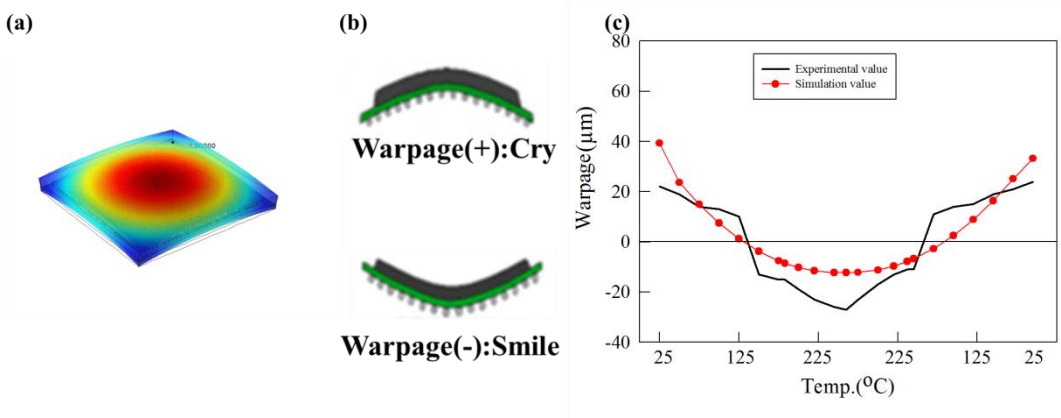


Fig. 2: (a) single unit simulation model ; (b)warpage cry(+) and smile(-) ; (c) experimental value and simulation value of shadow moire.

Contribution

This study successfully simulated the single unit warpage for the shadow moire measurement in Flip-Chip process. Fig. 2 illustrates single unit warpage of simulation model and results. This study found that the simulation value match the experimental value very well, which the trend of deformation is consistent. According to the aforementioned, this simulation method can be used to estimate the single unit warpage. Furthermore, it can help to improve process yield and keep the cost down on the production line.

Keywords: CTE, Single unit warpage, Flip-Chip, Shadow moire

References

[1] S. J. Oon, K. S. Tan, T. Y. Tou, S. S. Yap, C. S. Lau, and Y. T. Chin, "Warpage Studies of Printed Circuit Boards with Shadow Moiré and Simulations," in 2018

IEEE 38th International Electronics Manufacturing Technology Conference (IEMT), 2018, pp. 1-5

Efficient and accurate two-scale FE-FFT-based prediction of polycrystalline material behavior at finite strains

Christian Gierden[1], Julian Kochmann[1,2], Johanna Waimann[1], Bob Svendsen[1,3], Stefanie Reese[1]

[1]RWTH Aachen University, [2]MTU Aero Engines AG, [3]Max-Planck-Institut für Eisenforschung GmbH

christian.gierden@rwth-aachen.de, julian.kochmann@rwth-aachen.de, johanna.waimann@rwth-aachen.de, b.svendsen@mpie.de, stefanie.reese@rwth-aachen.de

In order to capture a complex heterogeneous material behavior in structural finite element simulations, the application of a two-scale simulation approach is required to account for individual microstructural effects. In this context, former studies [1] already show that the recently developed FE-FFT method (e.g. [2]) seems to be more efficient than the common FE² method (e.g. [3]). However, the computational effort for a two-scale simulation is still extremely high. In order to reduce this effort, more efficient methods, e.g. FFT-solvers in combination with model order reduction techniques [4], are necessary. We present an efficient FE-FFT-based simulation approach for the prediction of the local and overall mechanical behavior of polycrystalline materials, which is introduced by Kochmann et al. [5], and extend this simulation approach for finite strains and for more general microstructures.

The proposed solution scheme is decomposed into three steps: (i) pre-processing, (ii) processing and (iii) post-processing. In the pre-processing step a convergence analysis in terms of the macroscopic stress is performed by considering different discretizations and thus a different number of grid points in each direction (see Figure 1). The result of this pre-processing step is a minimal number of grid points that must be considered to obtain a solution with an error which is

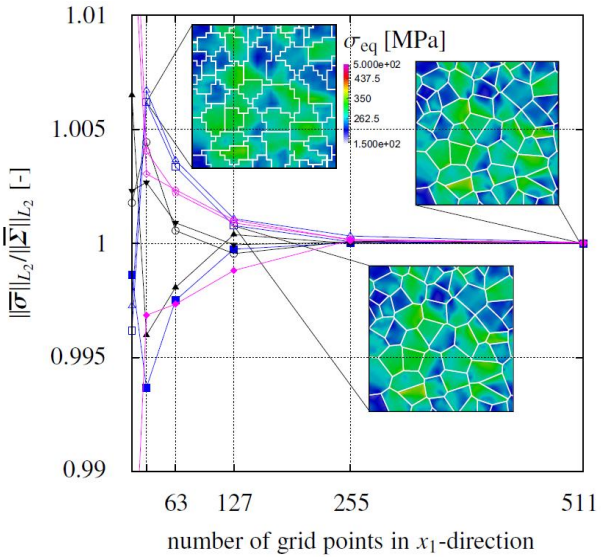


Figure 1. Error in the macroscopic stresses of different discretized microstructures for different load cases [5].

(compared to the converged solution) smaller than a prescribed tolerance. Secondly, in the processing step, the two-scale full-field simulation is performed using the coarse discretization of the minimal number of grid points. Within this simulation, the macroscopic strain tensor is stored at every macroscopic integration point of particular interest. Finally, in the post-processing step, highly resolved microstructure data are generated by applying the stored macroscopic strain tensor to a fine discretized microstructure.

In order to demonstrate the versatile use of the proposed approach, polycrystalline materials with different textures and different intrinsic anisotropy are considered. On this basis and as a first representative simulation, the micromechanical fields and the related overall material behavior of body-centered cubic (bcc) polycrystals are predicted for simple macroscopic boundary value problems.

References

[1] Prakash, A., Lebensohn, R.A., 2009. Simulation of mircomechanical behavior of polycrystals: finite elements versus fast Fourier transfomrs. Modelling and Simulation in Material Science and Engineering 17, 16pp.

[2] Kochmann, J., Wulfinghoff, S., Reese, S., Mianroodi, J.R., Svendsen, B., 2016. Two-scale FE-FFT- and phase-field-based computational modeling of bulk microscructural evolution and macroscopic material behavior. Computer Methods in Applied Mechanics and Engineering 305, 89-110.

[3] Smit, R.J.M., Brekelmans, W.A.M., Meijer, H.E.H., 1996. Prediction of the mechanical behaviour of nonlinear heterogeneous systems by multi-level finite element modeling. Computer Methods in Applied Mechanics and Engineering 155, 181-192.

[4] Kochmann, J., Manjunatha, K., Gierden, C., Wulfinghoff, S., Svendsen, B., Reese, S., 2018. A simple and flexible model order reduction method for FFT-based homogenization problems using a sparse sampling technique. Computer Methods in Applied Mechanics and Engineering 347, 622-638.

[5] Kochmann, J., Wulfinghoff, S., Ehle, L., Mayer, J., Svendsen, B. Reese, S., 2017. Efficient and accurate two-scale FE-FFT-based prediction of the effective materialbehaviour of elasto-viscoplastic polycrystals. Computational Mechanics 61, 751-764.

Diffusion-Kinetic Monte Carlo Methods for Neutral Transport in Plasma Edge Simulations of Nuclear Fusion Reactors

Bert Mortier[1], Martine Baelmans[2], Giovanni Samaey[1]

[1]KU Leuven, Department of Computer Science,
[2]KU Leuven, Department of Mechanical Engineering

bert.mortier@kuleuven.be

Economically viable nuclear fusion would provide a sustainable energy source for our planet, with nearly limitless resources and virtually no radioactive waste. A lot of progress is yet to be made, with ITER [1] and DEMO [2] reactors as the next important steps. The design of these reactors requires simulation of the plasma and its interaction with the solid components. Of these solid plasma-facing components, the divertor target receives the highest energy flux from the plasma. In a so-called detached regime, a relatively dense neutral mass cushion in front of the divertor limits the energy flux carried by ions towards the divertor target. To estimate these fluxes and the effectiveness of the cooling, simulations of the plasma edge are particularly important.

In a detached regime, the neutrals in the plasma edge traverse regions of high collisionality before being absorbed by the plasma in neighbouring regions of medium and low collisionality. The neutrals are modeled by a kinetic equation, discretized by a stochastic particle (Monte Carlo) method. In a high collisional regime, a kinetic simulation is expensive, since the Monte Carlo method requires resolving each individual collision. In that regime, however, a limiting fluid equation exists, which only considers mass, momentum and energy as a function of space and time. Such a fluid model is cheaper to simulate, but results in large errors when the collisionality is low.

We propose a modified simulation of the kinetic equation that uses a fixed time step Δt in which the individual collisions are aggregated into a diffusion step, resulting in a bounded simulation cost per time step. This aggregation is performed by taking a Brownian motion (diffusion) step of which the mean and variance correspond to the mean and variance of a kinetic simulation during the same time interval. Furthermore, potential large deviations by the first flight are resolved by taking an initial kinetic step, resulting in $O\left(\Delta t^{3/2}\right)$, $\Delta t \to 0$ convergence to the kinetic simulation. By including an additional kinetic step, an $O(\Delta t^3)$, $\Delta t \to 0$ convergence to the kinetic simulation is attained, for a small increase in simulation cost.

[1] Kukushkin, A. S., et al. "Finalizing the ITER divertor design: The key role of SOLPS modeling." *Fusion engineering and design*86.12 (2011): 2865-2873.

[2] Subba, F., et al. "Preliminary analysis of the efficiency of non-standard divertor configurations in DEMO." *Nuclear Materials and Energy* 12 (2017): 967-972.

Development of a simple ergodic stochastic representative volume element for heterogeneous materials with random geometry of microstructure

Dmytro Pivovarov [1], Kai Willner [1], Paul Steinmann [1]

[1] Chair of Applied Mechanics, Friedrich-Alexander University Erlangen-Nürnberg

dmytro.pivovarov@fau.de

Due to high computational costs associated with stochastic computational homogenization, the highly complex random material microstructures are replaced often by some simplified, parametric, ergodic and sometimes periodic models. This replacement is often criticized in the literature due to unclear error resulting from periodicity and ergodicity assumptions. In this work we propose an approach to design this kind of simplified models for heterogeneous materials with randomly distributed inclusions with random radii, which demonstrates a good agreement with full-scale non-ergodic simulations. Proposed model design is based on some assumptions: dominating role of volume fraction in determination of homogenized quantities, ergodicity assumption, and priority of the interparticle distances over other microstructural characteristics. Accuracy of the presented simplified model is validated through a numerical example.

Multi-uncertainty analysis of the indentation process of key engineering materials

T.L. Amaral, T. Doca[1]

[1]University of Brasilia, doca@unb.br

Indentation tests are often used to obtain surface properties, such as hardness [1], and can also be employed for the mechanical characterization of a material [2,3]. These tests require equipment with multiple known sources of uncertainty. For instance, the input of axial force is bound to the error of a loading cell while the displacement sensor is affected by disturbances in the servo-hydraulic system. These uncertainties contributes to the overall dispersion of the results, in this case, the depth and width of an indentation mark.

An assessment of the influence of these uncertainties is presented. The compression tests are performed using a MTS 809 and sample holder device. A sphere-to-flat contact configuration is chosen. Tests are carried-out in the both the elastic regime and after the onset of inelastic strains. The indentation marks are measured with a confocal laser microscope. Four different materials are analysed: CA6NM stainless steel, R3 grade offshore steel, Polycarbonate (PC) and a blend of PC and Acrylonitrile Butadiene Styrene (ABS).

The four sources of uncertainty studied are: i) variation of the Elastic modulus; ii) error of the loading cell; iii) error of the displacement sensor; iv) error of the measured dimensions of the indentation mark. The experimental data is compared to numerical predictions [4] and analytical results [5-6] to evaluate the correlation between these different types of analyses.

References

[1] H Chandler. Hardness testing. Cleveland: ASM International; 1999.

[2] MB Toloczko, ML Hamilton, GE Lucas. Ductility correlations between shear punch and uniaxial tensile test data. J Nucl Mater, 283 (2000)

[3] RK Guduru, KA Darling, R Kishore, RO Scattergood, CC Koch, KL Murty Evaluation of mechanical properties using shear-punch testing. Mater Sci Eng A, 395 (1–2) (2005)

[4] T Doca, FM Andrade Pires, JMA César de Sá. A frictional mortar contact approach for the analysis of large inelastic deformation problems. Int J Solids Struct; 51:1697–715 (2014).

[5] R Hill. The mathematical theory of plasticity.Oxford:Oxford University Press Inc.; 1950.

[6] KL Johnson, Contact mechanics, Cambridge University Press, 1987.

Adjoint Based Optimisation of an Internal Cooling Channel U-Bend

Jens-Dominik Müller [1], Oluadamilare Imam-lawal [1], Tom Verstraete [2]

[1]Queen Mary, University of London, Von Karman Institute for Fluid Dynamics

ghanem@usc.edu

Conjugate Heat Transfer (CHT) is a multidisciplinary problem which occurs when heat is transferred between a fluid and a solid. Numerical optimisation of CHT problems has mainly used gradient-free methods which is limited to a small number of design variables [1]. Alternatively, gradient-based optimisation can handle large design spaces, and are very economical if gradients are computed with the adjoint method. While the use of adjoint methods is common for single disciplines, it is a recent field of interest in CHT [2].

CHT problems may be solved in a partitioned manner where separate solvers are used for both domains and the exchange of boundary conditions between solvers is required [3]. The use of partitioned coupling and adjoint methods for CHT optimisation presents an interesting challenge as it requires the differentiation of the numerical solvers and their coupling. The exchange of boundary conditions and adjoint gradients between the solvers is dependent on the type of coupling method used. In this work, we make use of Automatic Differentiation (AD) to obtain adjoint gradients. The paper will present the application of AD to the solvers, as well as and the differentiation of the coupling boundary conditions, resulting in a consistent exchange of gradients between solvers.

We consider an optimisation problem in which the goal is to reduce the pressure loss in a U-Bend cooling channel [3,4]. This is achieved by performing a gradient-based optimisation to change the shape of the cooling channel. The results are obtained using the open-source structural solver CalculiX and the in-house flow solver STAMPS. The results show how the discrete adjoint method obtained using AD can be effectively combined with partitioned CHT methods to solve optimisation problems.

References

[1] Ping He and C.A. Mader and J.R.R Martins and K.J. Maki, “Aerothermal optimization of internal cooling passages using a discrete adjoint method." *AIAA*, (2018).

[2] K.T. Gkaragkounis and E.M. Papoustis-Kiachagias and K.C. Giannakoglou , “The continuous adjoint method for shape optimization in Conjugate Heat Transfer problems with turbulent incompressible flows." *Applied thermal Engineering*, 140 (2018), pp (351-362).

[3] T. Verstraete, F. Coletti, J. Bulle, T. V. der Wielen, and T. Arts. Optimization of a U-Bend for Minimal Pressure Loss in Internal Cooling Channels Part I: Numerical Method. ASME Journal of engineering for Gas Turbines and Power, 135:pp 051015, 2013.

[4] F. Coletti, T. Verstraete, J. Bulle, T. V. der Wielen, N. van den Berge, and T. Arts. Optimization of a U-Bend for Minimal Pressure Loss in Internal Cooling Channels – Part II: Experimental validation. ASME Journal of engineering for Gas Turbines and Power, 135:pp 051016, 2013.

System time-variant reliability-based structural design optimization of deteriorated truss bridges

Younes AOUES[1], Didier LEMOSSE[1], Eduardo SOUZA DE CURSI[1]

[1]Normandie Univ, INSA Rouen Normandie, LMN, France.

Younes.aoues@insa-rouen.fr

The CLASSE2 project focuses on the performance conditions of supply chains and the reliability of the logistic corridors of the Normandy region. The fluidity of logistics corridors depends mainly on the reliability of infrastructures transportations. Highway bridges are considered the most critical and vital links in any transportation network, where a full or partial failure of these infrastructures leads to decrease the operational efficiency of the network and can provoke serious economic impacts. These infrastructures undergo various degradation (decay, aging, corrosion, fatigue) due to the weather conditions, natural disaster, the increase in traffic of the last decades.

In the current economic context, design optimization is usually applied to cost reduction and to improve structural performances. The optimal design is generally searched by minimizing the structural cost and checking performance criteria and the design requirements. The reliability-based design optimization (RBDO) approach aims to find the best compromise between the structural cost and safety assurance [1]. The RBDO approach is based on considering uncertainties related to geometry, material properties and approximation models that affect the structural system.

Bridges are subjected to various deterioration processes that reduce their structural performance significantly during their long-term performance (e.g., decay, aging, corrosion, fatigue, etc.). The structural deterioration is a major problem for many companies and countries, where important costs are involved to maintain, repair or to replace the deteriorated structures. Therefore, when structures are subjected to degradation during their lifetime, the RBDO approach should consider the time-dependency of load and environmental fluctuations. This time-dependency can be considered by using a time-variant reliability analysis where load and environmental variables are modelled by stochastic processes [2]. However, the failure of the truss structures is devoted to several failure modes (i.e. several limit state functions) [3]. Thus,

the time-variant RBDO approach may consider the overall system reliability (i.e. a combination of several limit states) instead of the single component reliability (i.e. single limit state function).

This study presents a new methodology for the system time-variant reliability-based design optimization, where the system time variant reliability is estimated on the basis of the time-variant limit state functions. In order to alleviate the computational time of the RBDO procedure [4], the system time variant reliability analysis is decoupled from the optimization procedure. In other words, the proposed approach is based on transforming the system time variant RBDO problem into a sequence of equivalent deterministic design optimization sub-problems. This transformation is defined by the mean of optimal safety factors, linking the reliability requirement to the equivalent deterministic optimization. At the end of each sub-problem optimization, the reliability constraint is verified by performing a system time-variant reliability analysis. The safety factors corresponding to the target reliability level at the desired lifetime are calibrated by an inverse probabilistic approach. Finally, these safety factors are provided to the following sub-problem of the equivalent deterministic optimization and so on, until convergence. This approach is applied to find the optimal design of truss bridges subjected to degradation. The overall results indicate that the system performance of the optimized truss ensures the target reliability level during the whole structural lifetime.

REFERENCES

[1] Frangopol, D.M., Moses, F. 1994. Reliability-based structural optimization. Adeli H, editor. Advances in design optimization. London:Chapman Hall.

[2] Kuschel, N., Rackwitz, R. 2000. Optimal design under time- variant reliability constraints. Structural Safety 22(2): 113-27.

[3] Aoues, Y., Chateauneuf, A., Lemosse, D., El-Hami, A. 2013. Optimal design under uncertainty of reinforced concrete sturcutres using system reliability appraoch, International Journal for Uncertainty Quantification 3(6): 487–498.

[4] Aoues, Y., Chateauneuf, A., Benchmark study of numerical methods for reliability-based design optimization, Structural & Multidisciplinary optimization 2010;41(2):277–294.

Examining the Mutation Effect of SLC26A4 STAS Domain By Observing the Communication Between Secondary Structures

Hyun Joon Chang [1], Jae In Kim[2], Sungsoo Na[1*]

[1]University of Southern California

[2]Hyundai Steel Company

[*]nass@korea.ac.kr

The mutation of STAS domain within Pendrin (SLC26A4), a protein associated with the auditory system, causes typical auditory disorders such as Pendred syndrome (PDS) and DFNB4. In this study, we generated six mutated STAS domain models related to PDS, DFNB4, and PDS/DFNB4 as well as the wildtype model, and performed Molecular dynamics simulations to find the difference in equilibration conformation and fluctuation information. We used network analysis on a residue-residue scale to calculate betweenness centrality and edge betweenness, and further scaled up to secondary structures to reveal the communication map within the STAS domain. Our results showed that the communication signals generated by the mutated models are less clear than those of WT model.

Presenting Author, Second Author, Corresponding Author

New Vortex Identification Methods - Omega, Liutex/Rortex, Omega-Liutex

Chaoqun Liu [1]

[1]University of Texas at Arlington, Arlington, Texas, USA

cliu@uta.edu

Vortex is intuitively recognized as the rotational/swirling motion of the fluids, but a universally accepted definition of vortex is still not available. In thousands of research papers and almost all textbooks, vorticity tube/filament is regarded equivalent to vortex and the magnitude of vorticity is deemed the strength of vortex, which is a misunderstanding of the vortex nature since Helmholtz (1858). During the last three decades, a lot of vortex identification methods, including Q-, Δ-, λ_2-, λ_{ci}- criteria, have been developed. Most of these criteria are based on Cauchy-Stokes decomposition and/or eigenvalues of the velocity gradient tensor. Starting from 2014, the Vortex and Turbulence Research Team at University of Texas at Arlington (UTA Team) focus on the development of a new generation of vortex identification methods. A new Omega vortex identification method, which defined the vortex as a connected region where vorticity overtook deformation, was published in 2016 [Liu et al, New omega vortex identification method, Science China: Physics, Mechanics & Astronomy, 2016, 59(8): 684711]. The Omega method has several advantages: (1) easy to perform, (2) clear on physical meaning, (3) non-dimensional and normalized from 0 to 1, (4) robust to threshold change, (5) able to capture both strong and weak vortices simultaneously. In 2017 and 2018, a Liutex (previously called Rortex) vector was proposed by UTA Team to represent the local rigid rotational part of fluid motion, which is a mathematical definition with its direction as the local rotational axis and its magnitude as the rigid rotation strength [Liu et al, Rortex—A new vortex vector definition and vorticity tensor and vector decompositions Physics of Fluids 30, 035103 (2018); doi: 10.1063/1.5023001]. Liutex/Rortex is

a new physical quantity with scalar, vector and tensor forms exactly representing the local rigid rotation of fluids. Meanwhile, a decomposition of vorticity to a rotational part namely Liutex/Rortex and an anti-symmetric shear part (RS decomposition) was introduced in 2018 and a velocity gradient tensor decomposition to a rotation part (R) and a non-rotation part (NR) which could be further decomposed as pure shearing (PS) and stretching and compression (SC) was given in 2019 [Gao and Liu, Rortex based velocity gradient tensor decomposition, Physics of Fluids, Phys. Fluids **31**, 011704 (2019); https://doi.org/10.1063/1.5084739] as a counterpart of Cauchy-Stokes decomposition. Later in early 2019, a Liutex/Rortex based Omega method called Omega-Liutex [Dong, Gao and Liu, New normalized Rortex/vortex identification method, Physics of Fluids 31, 011701 (2019); doi: 10.1063/1.5066016] was developed, which combines the advantages of both Liutex and Omega methods. These breakthroughs in the development of vortex science by UTA Team are classified as a new generation of generation of vortex identification methods. The critical problems for vortex identification concern with the vortex core location, vortex core size, vortex boundary and size, absolute vortex strength, relative vortex strength, mixture of strong and weak vortices, vortex rotation axes, etc. Only the new third generation of vortex identification methods can answer these questions while all the other vortex identification methods fail to answer all questions except for part of the first one (approximate vortex boundary when the threshold is extremely small). The talk will introduce the new vortex identification methods including Omega, Liutex/Rortex, Omega-Liutex. **A numeber of computational examples by using the new vortex identification methods for flow transition and turbulence will be reported.**

Presenting Author, Chaoqun Liu, cliu@uta.edu

Multi-scale and Multi-physics challenges for Future Aircraft: A Hierarchical Approach

Paul G. Tucker [1]

[1]University of Cambridge

Pgt23@cam.ac.uk

The various multi-scale and multi-physics modelling needs of future aircraft are discussed. In a hierarchical fashion both the handling of the inevitable turbulent flow and geometry are considered. The latter is necessary to help more economically deal with the increasingly coupled nature of many aerodynamic problems and also the drive towards considering ever increasing levels of geometrical complexity. The proposed unified framework could be exploited all the way though initial fast preliminary design to final numerical test involving various bespoke combinations of hierarchical components.

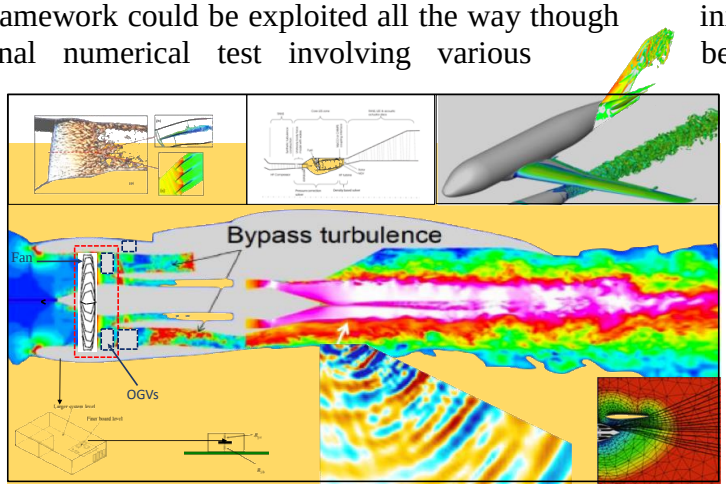


Figure 1. Multi-scale elements of modern aircraft and their engines.

The aircraft engine is inherently a multi physics system. Fuel is burned. This generates aerodynamic forces which in turn drives the turbine and ultimately creates aerodynamic thrust. The combustion system in a modern aircraft engine is also inherently multiscale but this time as a sub-system. Its design intent is to generate large scale turbulence which itself generates subsequently smaller turbulent scales. Fuel is mixed into these scales the fuel is broken down into droplets. The combustion process, from the ignited droplets, results in a flame front. This fine front has wrinkling. The smaller more complex this wrinkling the more efficient the combustion process. Efficiency of the combustion process and the aerodynamics together is of clearly of vital importance with respect to global warming. By 2025 there will be around 1 billion tonnes of annual CO_2 emissions from aircraft alone. Naturally the aircraft engine is tremendously powerful and this results in the generation of substantial aerodynamic noise. The reduction of this noise is the second major aerospace priority in the US and Europe. The aeroelastic response of the components in the aircraft system at a wide range of scales is also an area of considerable importance. Hence, the system is clearly multiphysics. The engine itself is intrinsically a multi scale system. For example, the diameter of the engine is around 2 m and this roughly corresponds to the diameter of the fan at the front of the engine. Figure 1 shows selected multi-scale elements of modern aircraft and their engines. Most of the thrust comes from the fan which for the purposes here can be considered as *e*ffectively a propeller. After the fan there are blades that compress the air *leading to the combustor*. The energy liberated by this drives the turbine

which in turn drives the fan, any residual energy is used as thrust coming out of the back of the engine in the form of a jet - called the propulsive jet.

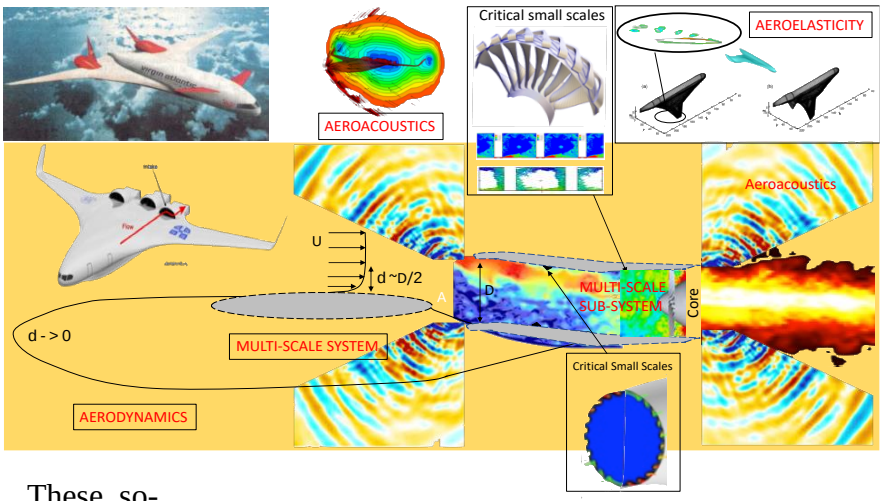


Figure 2 Multi-scale elements of future blended wing-body aircraft.

Since the fan also compresses the air, like the compressor, there is a risk of the air flowing backwards. This is often mitigated by using fine intricate structures embedded in the shroud geometry above the tips of these components. These so-called casing treatments are shown in figure 2 (top row, 3rd element along from the left). The casing treatments can range from geometries involving simple grooves, to far more complex multi-scale configurations. The disparity in scale between the fan and these grooves is many orders of magnitude. Figure 3 shows the core of an engine. Consisting of the compressor stages, combustor and subsequesnt turbine. The turbine is also, in itself, is a problematicaly multi-scale system. The largest disparity in geometrical scale is that of the blade chord (or span) to the fine holes that shield the surface from hot gasses from the combustion. This ratio is around 1000. Suface roughness from wear is important to the turbine blade increasing surface skin friction by 80%. The inside of the turbine balde has complex multiscale cooling eleements. The balde extremeities also have coplex seals. All these elements are shown in Figure 3.

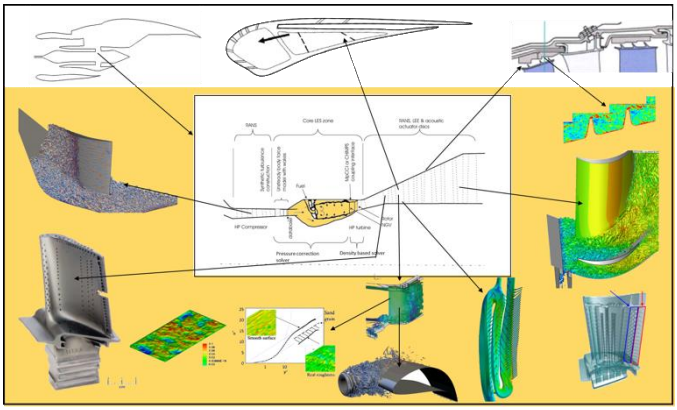


Figure 3. Multi-scale elements of turbine.

Here it is proposed to deal with the above noted multi-scale and physics challenges using hierachical modelling for both turbulence and geometry. For futurue aircraft this is especially important since the airframe and engine are becoming ever more closely integrated. This can be seen to a degree in the next generation as shown in Figure 1 and far more fully in the future – see Figure 2.

Probabilistic Design Optimization for CO2 Storage with Leakage Risk Control

Ben Mansour Dia[1] and Bilal Saad[2]

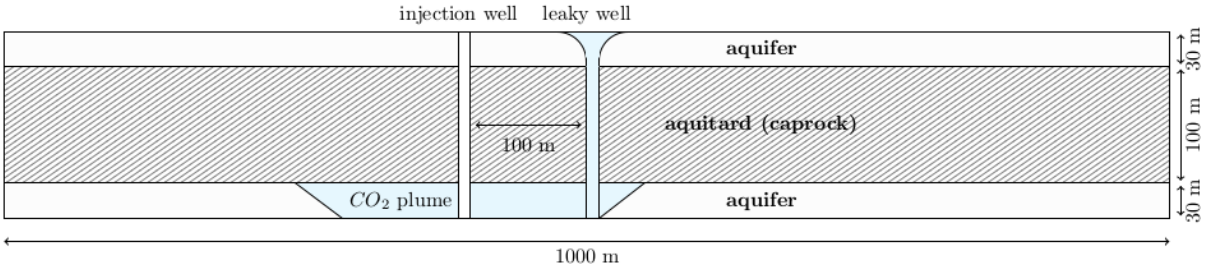
[1]CPG, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

[2]Baker Hughes Research Center, Dhahran Techno Valley, Dhahran, Saudi Arabia

diabenmansour@gmail.com

The physical process of CO2 injection in geologic reservoirs, including solubility trapping, is a non-isothermal two-phase two-component flow in porous media, which is governed by a system of coupled nonlinear partial differential equations [2]. In this model, the water-rich phase (brine) and the carbon dioxide-rich phase (CO2) consist of two components (water and CO2 component), as the solubility of the components in the phases has to be taken into account. Local equilibrium phase exchange of the components in the phases is assumed to hold. To close the system, the fluid properties of CO2 are calculated as functions of pressure and temperature.

For simulations purpose, a reservoir composed of two aquifers separated by an aquitard is considered. The leaky well is modeled as a porous medium with higher permeability compared to the rest of the formation. We count the effect of uncertainties in reservoir porosity, reservoir absolute permeability, and permeability of the leakage well, on the model response. Also, we consider spatial heterogeneity only through the different layers according to different geological media, and we count the changes in fluid properties of CO2, and that the CO2 and brine fluid properties (e.g., density and viscosity) depend on the aquifer conditions, the temperature, the CO2 pressure, the brine salinity, and the mass fraction of CO2 in brine.



In the talk, we present scenario where CO2 is injected to be stored in the lower aquifer and the injected CO2 spreads within the aquifer and once it reaches the leaky

well, it connects the two aquifers and rises to the shallower aquifer. The following sketch summarizes the model geometry and illustrates a 2D section of the 3D domain. We address an optimal experimental design problem under uncertainties, [1,3], with the main objective of searching the optimal injection rate of CO2 for the learning of the leakage rate in order to consistently maintain the harmful leakage risk.

References

[1] C. Thimmisetty, P. Tsilifis, R. Ghanem, Homogeneous chaos basis adaptation for design optimization under uncertainty: Application to the oil well placement problem. *Artificial Intelligence for Engineering Design, Analysis and Manufacturing (2017), 31, 265–276.*

[2] B. M. Saad, A. Alexanderian, S. Prudhomme, O. M. Knio, Probabilistic modeling and global sensitivity analysis for CO 2 storage in geological formations: a spectral approach. *Applied Mathematical Modelling 53 (2018) 584–601*

[3] J. Beck, B. M. Dia, L. F. R. Espath, Q. Long, R. Tempone, Fast Bayesian experimental design: Laplace-based importance sampling for the expected information gain. *Computer Methods in Applied Mechanics and Engineering 334 (2018) 523–553.*

Development of Multiscale Multi-physics Based Modelling and Simulations with the Application to Precision Machining of Aerofoil Structures

Kai Cheng[1], Yizhi Shao[1] and Rodrigo Bodenhorst[1]

[1]Brunel University London

Kai.cheng@brunel.ac.uk, Yizhi.shao@brunel.ac.uk

Multiscale multi-physics based modelling and simulations are getting more and more interest by the industry and research community particularly in the context of increasing demands for high precision manufacturing and complex production environment. With the development of multiscale multi-physics based modelling and simulation, it will enable effective and efficient optimisation of the manufacturing process and further improvement of the production in terms of quality, costs, shortest delivery and overall competitiveness. In this paper, some basic models and analysis using multiscale multi-physics modelling are presented and discussed. Furthermore, the possibility of adopting the multiscale multi-physics modelling and simulation to the virtual machining system is evaluated, and further supported with an industrial study case study on Abrasive Flow Machining (AFM) of integrally bladed rotors (IBR) using the modelling and simulation techniques above.

An Investigation of Stepwise Crack Tip Advancement

Yanan Sun[1], Bin Chen[2], Michael G Edwards[1], and Chenfeng Li[1]

[1]Swansea University

[2]Imperial College London

966781@.Swansea.ac.uk

This research focuses on stepwise crack tip advancement associated with hydraulically induced fractures, which are observed both in the field and in experiments and reported in the numerical fracture modelling literature.

A numerical model of hydraulic fracture in porous media is established. The finite element method is employed to solve the fully coupled equation system, which includes rock deformation, fluid flow in both the fracture and rock matrix and fracture propagation. To reproduce the stepwise phenomenon, a special time stepping scheme is used, which allows for multiple incremental fracture advancement within a time step according to a cohesive stress constraint. With the model, the contributing factors to the stepwise phenomenon are studied, and a numerical sensitivity analysis of this phenomenon is presented.

The contributing factors are summarized, including Young's modulus, Poisson's ratio, Biot's coefficient, Biot's modulus, rock porosity and permeability, viscosity, injection rate and fracture toughness. Among all the factors, Young's modulus, permeability, injection flow rate, fluid viscosity and fracture toughness are found to be predominant. A further key contributing factor is that the velocity of solid deformation is much faster than fluid deformation. This study helps to understand the influence of different factors to the stepwise phenomenon and provides possible explanations behind this phenomenon.

Dynamic Analysis of a Multi-Contact Problem

Using Simplified Models to Study of the Influence of Clearances on Contact Forces

Thomas Catterou [1], Victor Blanc[1], Guillaume Ricciardi[2],

Stéphane Bourgeois[3], Bruno Cochelin[3]

[1]CEA Cadarache, DEN/DEC/SESC/LECIM, F-13108 Saint Paul Lez Durance, France

[2]CEA Cadarache, DEN/DTN/STCP/LTHC, F-13108 Saint Paul Lez Durance, France

[3]Aix Marseille Univ., CNRS, Centrale Marseille, LMA, Marseille, France

victor.blanc@cea.fr

The purpose of this paper is to show the efficiency of a simplified multi-body system in order to analyze dynamic response of a multi-component system with clearances. Initially, a 2D multi-contact model based on beam finite element model and a modal basis reduction has been developed in order to compute the global response of a nuclear fuel subassembly submitted to a shock. The assessment of contact forces that occurs between sub-components must be conservative, but, as already observed in the literature, results show that the evolution of the contact forces with initial joint clearances is clearly non-linear and presents a maximum for small gaps values, what is counter-intuitive.

In order to reduce computational costs and to analyze the effects of initial joint clearances by a parametric study, a simplified spring-mass system is presented in this paper. Characteristics of the simplified model are chosen using an analysis of the spectral response of the finite element model. The simplified model is dimensionless using first modes of vibration of the components.

First, we observe that physical phenomena, which causes the chaotic response described by the finite element model are very well reproduced by the simplified multi-body system. In addition, as observed with the finite element model, contact forces present a maximum for small values of the initial gaps. Characteristic times of compression waves and of local contacts oscillation are very close to the detailed model.

Secondly, phenomenology of the forces transfer between masses is analyzed, and related to the initial gaps values. The displacements are also analyzed, and their evolution

allow us to understand phenomenon that causes the increase of the contact forces for small gaps values. This result shows the interest of such simplified model in order to explain complex physical phenomena occurring inside these structures.

A phase-field damage model with micro inertial effect for dynamic failure of quasi-brittle materials

Lu Hai[1], Jie Li [2]

[1]Tongji University

tjhailu@tongji.edu.cn

[2]Tongji University

lijie@tongji.edu.cn

The prediction of the structural response and failure under dynamic loadings such as blast and impact is of particular importance to the design of concrete structures. Various theoretical models, based on the plasticity theory, fracture and damage mechanics, etc., have been developed to characterize the dynamic mechanical behavior of concrete. Compared to quasi-static loading, quasi-brittle materials subjected to high-rate loading exhibit the rate-dependency due to the inertial effects at multiple scale levels. The resistance, failure mode and crack pattern are sensitive to the strain rate, which is the main challenge when developing a continuous model for dynamic failure.

Recently the phase-field method for damage and failure in solids has attracted extensive theoretical and computational investigations. With extension to quasi-brittle failure, the researches indicate that the phase-field model can predict the global responses of concrete structures under static loads accurately, e.g. load-displacement curve and crack path. However, the phase-field model for dynamic failure of concrete still remain an open and challenging issue. The rate-dependency of materials is not considered in existing models.

To overcome the above problem, we introduce the micro inertial mass to consider the physical mechanisms of strain-rate sensitivity in this contribution. Based on Hamilton principle, a novel phase-field damage model with microscale inertial effect is proposed. The model performance is tested with two sets of numerical examples including compact tension tests and spall tests of concrete at high strain rate. Good agreement is achieved with numerical results and experimental results; and particularly the rate-dependency of concrete subjected to high-rate loading can be investigated with this model.

Two-scale phase field modeling of damge and fracture for disordered media

Ye Feng [1] and Jie Li [2]

[1] Tongji University, Shanghai, China

1710181@tongji.edu.cn

[2] Tongji University, Shanghai, China

lijie@tongji.edu.cn

As a continuum field description, phase field method provides possibility to describe the complex evolution of crack fronts without any extra computational efforts to track crack path. In phase field modelling, an order parameter is used to describe the local damage state of material. The order parameter is taken zero in intact phase and some positive value in "broken" phase. The key idea is to regard damage and fracture evolution as a process that spontaneously reduces the total free energy, which can be written as a functional of displacement field and order parameter field (or phase field). This idea can be conveniently implemented in finite element method after using variation principle.

In principle, phase field method is valid at any scale as long as the "infinitesimal" volume in the model can still be regarded as macroscopic element that contains huge number of particles. However, a very fine mesh is required to capture the diffusion of crack surface, because the thickness of the real crack surface is only a few molecules radius width. In practical, the thickness of crack is controlled by a numerical parameter and the surface energy density, which related to the total free energy minus elastic energy, is controlled as constant. A variety of phase field models have been proposed for ideal brittle homogenous media, where the surface energy density (or fracture strength) is a constant field. However, many practical materials, such as concrete, bone and ceramics, are heterogeneous and the fracture strength should be treated as a random field. The macroscopic mechanical behaviors are quite different between homogenous material and random media.

This talk will describe recent efforts at developing a two-scale phase field method of damage and fracture for discorded media, where the fracture strength is assumed as a random field with a very small correlation length. A discrete lattice model is introduced as a bottom model to derive the probability information of "damage potential" which is part of the total effective free energy. Then a macroscopic phase field model is developed

based on the information given by bottom lattice model. Numerical examples are given to show the property of the proposed method. The results show that the proposed method can reproduce phenomenon such as crack surface roughening and the random behavior in force-displacement curve.

The Refined Algrithm of Generalized Probability Density Evolution Equation Based on Reproducing Kernel Particle Method

Dan Wang [1,2] and Jie Li [1,3]

[1]Tongji University

[2]wangdan1995@tongji.edu.cn

[3]lijie@tongji.edu.cn

The generalized probability density evolution equation (GDEE) is a partial differential equation governing the evolution of the joint probability density function (PDF) of the response of interest and the source random variables, which holds for both linear and nonlinear stochastic dynamic systems. It's worth mentioning that the randomness involved in the initial conditions, excitations and structural properties can be taken into account simultaneously in the GDEE. Besides, the dimension of the GDEE is only dependent on the dimension of the quantity of interest, and nothing to do with the dimension of the stochastic dynamic system itself. The traditional numerical solving process of the GDEE, referred to as the probability density evolution method (PDEM), has been systematically developed, which has been applied to many areas, e.g., structural system reliability evaluation and stochastic optimal control, etc.

The key factor limiting the accuracy and efficiency of the tradition PDEM is the number of representative points required. On one hand, to alleviate the problem of mesh sensitivity, a large number of representative points should be selected. On the other hand, the step of deterministic analysis is computationally expensive to implement, especially for a complex structure involving high dimensionality and strong nonlinearity.

This talk will describe recent efforts at developing a numerical method for overcoming the above limitations, named the refined algorithm based on reproducing kernel particle method (RKPM), in which a surrogate model method and the PDEM are combined. By this method, the instantaneous probability distributions of the quantities of interest can be obtained. The problem of mesh sensitivity is settled well, and the accuracy is relatively high. Besides, the computational efforts are considerably reduced. The accuracy and efficiency of this method is verified by some numerical examples.

Data-Drive Approaches in Predicting Premixed Reactive Flow

Mohsen Ayoobi [1] and Ali Takbiri-Borujeni [2]

[1]Wayne State University and [2]West Virginia University

mohsen.ayoobi@wayne.edu, ali.takbiriborujeni@mail.wvu.edu

Complex interplays of different physical phenomena including ignition, chemical kinetics, turbulence, etc. make the computational simulation of combustion-related applications challenging in practical cases and therefore, researchers have to overlook some details and rely on simplistic models. For example, in order to decrease the computational expenses (memory and time), one may have to disregard the detailed chemistry, or filter the flame interactions with the flow and eddy structures at smaller scales. Such assumption limit the combustion-related applications that can be simulated with confidence in their accuracy. This study aims at employing Artificial Intelligence (AI) and more specifically Machine Learning (ML) techniques to predict combustion flame behavior. It is anticipated that the application of ML techniques will eventually reduce computational expenses significantly without having to sacrifice accuracy.

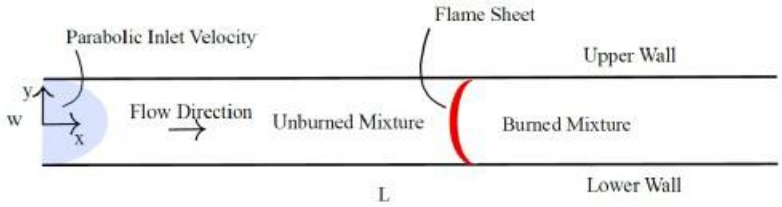


Figure 1: Schematic of the simulation domain

In this work, premixed combustion of two fuel mixtures at stoichiometric level ($\emptyset = 1$) and two different inlet velocities are simulated at micro scale channels (see Figure 1) with detailed chemistry. Details about the operating conditions for these cases are presented in Table 1. Here, w = 2 mm and L = 20 mm are the width and length of the channel, respectively. The simulation domain has the width of 1 mm with an axis-symmetric boundary condition on the lower wall.

Table 1: Variations of fuel mixture and inlet velocity for the selected cases

Case Number	Fuel Mixture	Inlet Velocity (m/s)
Case 1-1	30% CO, 5% CH_4, 65% H_2	1
Case 2-4	40% CO, 10% CH_4, 50% H_2	4

The simulation data, including flow and chemical properties at all grid cells in the computational domain, is separated into two sections: the first section with the largest amount of data (80% of the data) is used to train a Feedforwarding Artificial Neural Network (ANN) model, and the remaining 20% of the data is used to test validate the predictive capabilities and the robustness of the data-driven model.

The ANN model is tested by predicting simulation results at selected time steps that are not seen in the training procedure. Results indicate that it is plausible to train physics-based machine learning algorithms to predict reactive flows with significant reductions in simulation costs. For example, Figure 2 illustrates temperature distribution in the computational domain for Case 2-4 at time 8 ms, where direct numerical simulation (DNS) results are compared with those predicted by the data drive proxy (DDP) model.

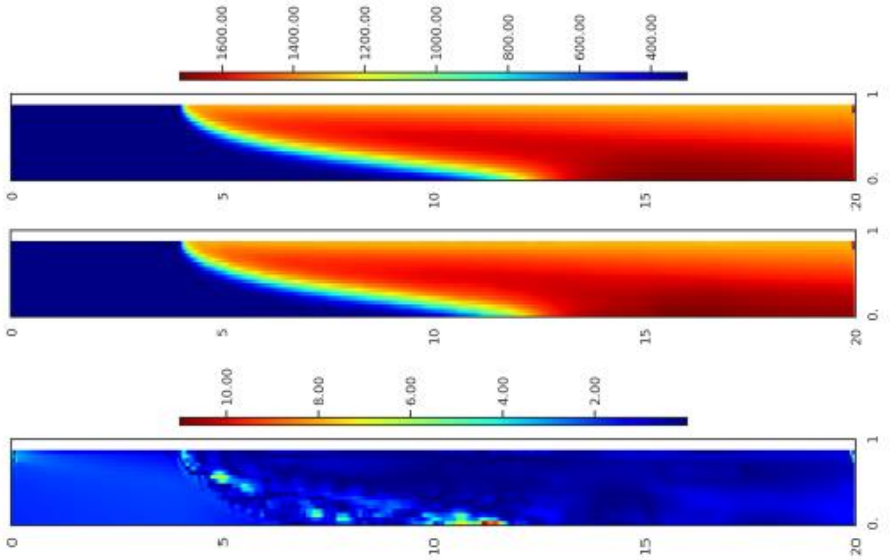


Figure 2: Comparison between temperature (K) predictions via DNS and DDP (Case 2-4 at time t = 8 ms). DNS (top), DDP (middle), and Errors % (bottom)

Results from this work illustrate an overall agreement between predictions from the DDP model and the DNS data. However, there are discrepancies to be addressed. These discrepancies are more considerable at the flame front, where the gradients are larger. For example, heat release rate and temperature experience a very large gradient across the flame front. With providing information about these gradients into the training procedure, such deviations can be reduced in future studies.

Comparisons of direct numerical simulation and penalized models to compute the flow in a porous-fluid system

Charles-Henri Bruneau [1], Didier Lasseux[2], Francisco Valdés-Parada[3]

[1]Univ. Bordeaux IMB, INRIA MEMPHIS, CNRS UMR5251, Talence 33405, France

bruneau@math.u-bordeaux.fr

[2]Univ. Bordeaux I2M, CNRS UMR5295, Talence 33405, France

[3]UAM , Mexico D.F. 09340, Mexico

For more than fifty years now, numerous analyses have been dedicated to the modeling of a porous medium-fluid system, either deriving a boundary condition at the interface or using a simplified model within which the porous medium is taken into account using a penalization method in order to avoid numerical simulation of coupled equations in the fluid and in the porous medium without knowing the appropriate conditions at the interface.

In this work, the porous medium is a large rectangle made of many particles close to each others and the aim is to compute accurately incompressible flow inside and outside the porous medium. The flow is first computed by solving the Navier-Stokes equations in the fluid domain. In a second step, the porous zone is replaced by an homogeneous medium taking into account its properties. Several models are proposed adding a penalization term inside the momentum equation and results are compared to those obtained by direct numerical simulation.

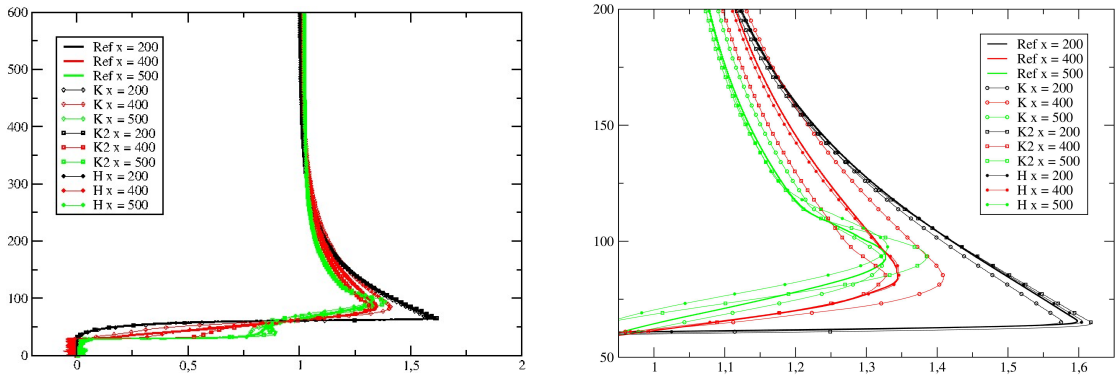
The Navier-Stokes equations are approximated by an accurate finite differences scheme and solved by a multigrid procedure involving several grid levels. The code is highly parallelized with MPI directives.

The models and the results are carefully analyzed to see which penalized model yields results closest to those obtained by the direct simulation. In particular the flow inside the porous medium is scrutinized and the velocity profiles are provided in the whole domain to highlight the impact of penalization approach close to and far from the porous zone.

To get the penalized models a term $\varepsilon\mu H(U)^{-1}U$ is added to the momentum equation where ε is the porosity of the porous medium, μ is the fluid viscosity and H is a tensor

which can depend on the velocity U. The simplest model (K) is obtained while considering H(U)=kI where k is the intrinsic permeability of the porous medium and I the identity tensor. A second order model (K2) with a quadratic term of the velocity can be easily derived and a more complex model (H) depending on the local Reynolds number and on the orientation of the pressure gradient inside the porous medium, can be used to improve the approximation.

The three models are compared to a direct numerical simulation (DNS) of Navier-Stokes equation in the fluid domain between the solid particles and outside the porous medium rectangle that is immersed in the fluid domain. The results are compared for three regimes: steady flow, chaotic flow and turbulent flow increasing the Reynolds number. The results show that for the two first cases the penalized models give a good approximation but not in the third case. This is due to the strong normal velocity coming in front of the porous rectangle that enters too fast inside the porous medium. Fortunately it is possible to modify the K model taking into account the local velocity inside the porous rectangle to get a very good approximation in turbulent case.



Vertical velocity profiles at three locations in x-direction for Re=100. The three models are compared to a reference flow obtained by DNS computed on a much finer grid.

The penalized models will be presented in details at the conference and a thorough discussion of the results will be conducted to convince the audience of the ability of the penalized models that are much cheaper than the direct numerical simulation.

Machine Learning-based Approach for Predicting Defects under Uncertainty in Sheet Metal Forming Processes

P.A. Prates [1], M.A. Dib [2], N.J. Oliveira [2], A.E. Marques [1], M.C. Oliveira [1], J.V. Fernandes [1], B.M. Ribeiro [2]

[1]Centre for Mechanical Engineering, Materials and Processes (CEMMPRE), University of Coimbra

[2]Centre for Informatics and Systems of the University of Coimbra (CISUC), University of Coimbra

pedro.prates@dem.uc.pt

Recently, there has been an increasing use of Machine Learning (ML) algorithms in a variety of engineering tasks. In fact, the vast majority of true Machine Learning users are not experts in Computer Engineering, Algorithms or Mathematics. They are professionals, often engineers working in other fields such as Mechanical Engineering, who want to make the best use of ML algorithms to solve real problems, to which the more traditional algorithms cannot completely respond.

An ML-based approach is proposed to extract information from a sheet metal forming processes, exposed to some sources of scatter, to enable the prediction of defects. The motivation is to reduce the costs and the time spent in the production of defective sheet metal components, i.e. contribute to improve the industry's efficiency. ML techniques are used assuming that they can build models able to generalize well in unseen data. In this context, an empirical analysis of performance of ML techniques is conducted, considering single and ensemble classifiers. These are trained using datasets populated with numerical simulation results of two sheet metal forming processes: U-Channel and Square Cup. Since these processes present distinct features, different types of defects were considered for each one. Each type of defect is studied separately using a binary classification. Moreover, the datasets are generated for each forming process, for three steels with distinct mechanical properties. For a given type of defect, most single classifiers show similar performances, regardless of the material. The fact that ensemble predictive models present relatively high performances, combined with the possibility of reconciling model bias and variance, offer a promising direction for its application in industrial environment.

On the universality of the Strouhal law for High Reynolds number bluff bodies with flow control

Avraham Seifert [1]

[1]Tel Aviv University

seifert@eng.tau.ac.il

In this paper I shall review recent near wake data obtained from a few flow control experiments related to bluff body flow control. In these experiments the main aim is drag reduction and vortex shedding when present is both a source of drag, but can also be used as an indicator for the success of the flow control effort and for drag reduction success. The relationship between natural vortex shedding and forced actuation is studied in detail from both surface steady and unsteady pressures and near wake velocities. It is shown that the classical Roshko results and scaling holds also for controlled wakes. Frequencies above the natural vortex shedding frequencies, especially with 3D actuation, are very effective for separation control and reduction of both surface pressures and wake unsteadiness, along with drag reduction.

Quantified Relationship between Properties of Fresh Self-compacting Concrete and Workability Test Performance

Sizeng You [1], Ashutosh Bhokare[1], *Chenfeng Li[1]

[1]College of Engineering, Swansea University, UK

* Corresponding author: c.f.li@swansea.ac.uk

Self-compacting concrete, known as SCC, has been continuously growing since its invention in 1980s. This type concrete could flow freely under its own weight, which is the most outstanding character. Nowadays, due to the massive production and wide application, a more accurate and quantified understanding on SCC rheology is highly required. The study on this topic has lasted for decades, and it's accepted that flow behavior of fresh concrete can be captured by Bingham Model. Despite of this consensus, a reliable solution to obtain involved parameters of SCC is still absent. Researchers have tried different methods including the analytical, experimental and numerical solutions[1,2,3], but no agreement is reached yet. Instead, the industry chooses to rely on the indicative measures of some robust workability tests.

To improve this situation, a systematic study by numerical simulation was carried out to investigate the flow performance of fresh SCC in standard workability tests. The tests include slump flow test, V-funnel test, modified-cone outflow test and inverted-cone outflow test. For the parameters of Bingham model, yield stress varies from 10 Pa to 100 Pa, and viscosity varies from 10 Pa•s to 100 Pa•s. Before carrying on mass simulation, models for different workability tests require careful design. To achieve better accurary, structured mesh is applied to all models. The most important work in the setup is to decide the element size, which will affect not only computational efficiency but also the model accuracy. The satisfied element size should pass the convergence check and match the accuracy requirement of certain workability test. Following these chosen setups, a batch of simulations were performed and a large set of data was collected recording the whole flow process of all simulations.

Analysis of this set of data shows that the measures of 4 workability tests vary monotonically with either yield stress or viscosity. Therefore, it's known that the 2 parameters of Bingham Model can be uniquely determined by measurements of two different tests. Following this idea, a specific graph depicting the such unique quantified relationship is designed. Considering that the latter 3 tests all belong to outflow tests, 3 test combinations are chosen for graph plotting including (slump flow test, V-funnel test), (slump flow test, modified-cone outflow test) and (slump flow test, inverted-cone outflow test). It's found that all of the 3 graphs share the same pattern with only scale difference as shown in Fig.1. In the figure, τ_0 denotes yield stress, μ denotes viscosity, D denotes spread diameter of slump flow test and t_n denotes discharge time of V-funnel test. And they are easy to be used in practice. Whatever concrete properties are known or measurements of workability tests are known, values of the other can be quickly located on these graphs.

At last, an application example of this graph is performed by simulating construction of a 6-meter high diaphragm wall. According to in-situ test result, the property variation of placed SCC is determined referring to the corresponding graph. In order to shown construction process, 9 representative parameter combination are chosen. The distribution of 9 type different SCC shows the concrete flow pattern in diaphragm wall, as shown in Fig. 2. In the figure, one colour mean one type of concrete and subfigures are taken from cross setions of this diaphragm wall. The number on each subfigure is the distance from this section to one side of the wall.

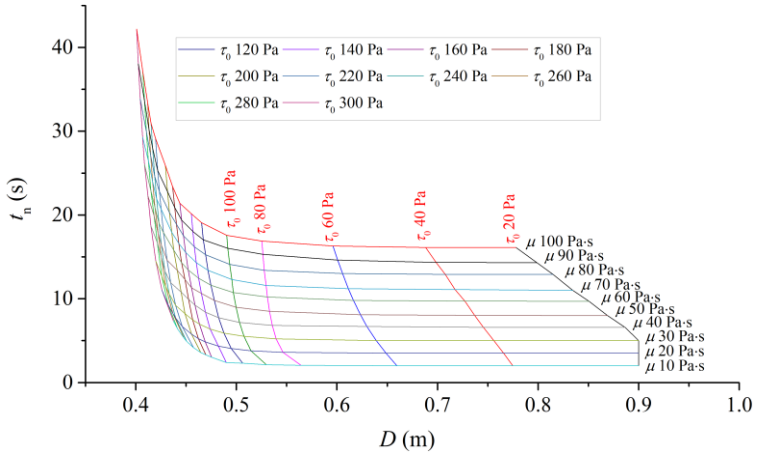


Fig.1 Relationship between (τ_0, μ) and (D, t_n)

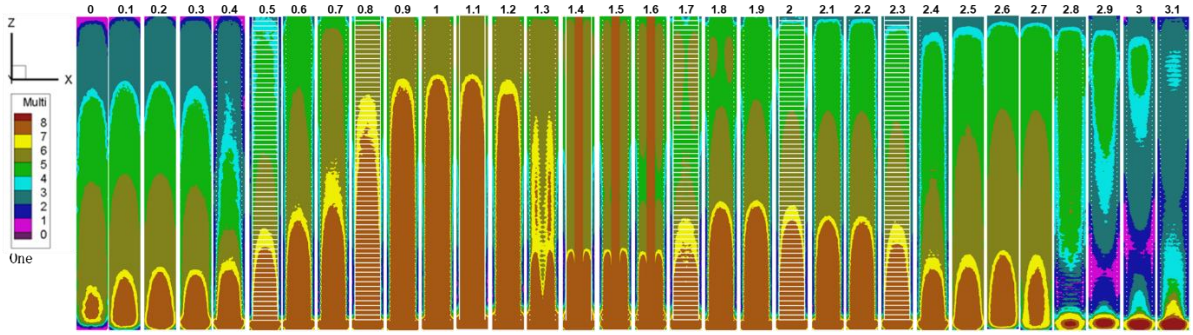


Fig.2 Concrete Distribution in Diaphragm Wall

References

[1] L.E. Brower and C.F. Ferraris. Comparison of concrete rheometers. *Concrete International*, 25(8), 41-47, 2003.

[2] N. Roussel and P. Coussot. Fifty-cent rheometer for yield stress measurements: from slump to spreading flow. *Journal of rheology*, 49(3), 705-718, 2005.

[3] A. Bouvet, E. Ghorbel and R. Bennacer. The mini-conical slump flow test: Analysis and numerical study. *Cement and concrete research*, 40(10), 1517-1523, 2010.

Robust Flame Frequency Response Identification via a Multi-Fidelity Approach

Shuai Guo[1], Camilo F. Silva, Wolfgang Polifke

Technical University of Munich

[1]guo@tfd.mw.tum.de

The frequency response of a linear time-invariant (LTI) system plays a crucial role in the analysis of system dynamics and corresponding system stability. A naive approach to obtain the frequency response of an LTI system is by harmonically exciting the system at many discrete frequencies and obtaining their responses. This method is highly accurate due to the high signal-to-noise ratio (SNR), but is generally not feasible in CFD simulations of complex systems, because of the high computational cost. An alternative method involves broadband excitation combined with advanced system identification analysis. This method, termed SI, provides the complete frequency range of interest of the system response with one single transient simulation. However, the SI method may introduce uncertainties on the identified frequency response due to the limited length of the simulated time series (of the order of tenth of seconds) and the associated low SNR when a strong noise level is present.

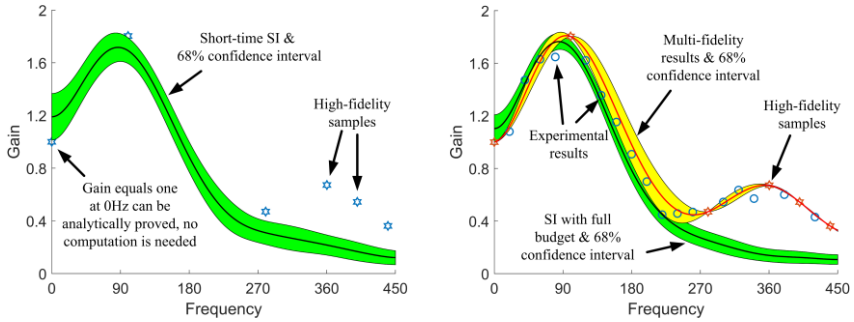
In this study, we propose a multi-fidelity approach to exploit the strengths of the two aforementioned methods to achieve more globally accurate and robust frequency response identification. We aggregate the frequency response identified from a short time broadband excitation (low-fidelity), with responses from harmonic excitations at a few frequencies (high-fidelity). This is realized via *Hierarchical Gaussian Process* (HSP), which takes the low-fidelity results as the global trend in the Gaussian process model of the high-fidelity function. To derive the prediction uncertainty of the multi-fidelity results, firstly, we adopt the regression version of the Gaussian Process, which allows to specify the uncertainties of the high-fidelity training samples and does not enforce interpolation of such samples. In addition, we propose a bootstrapping strategy to propagate the uncertainties associated with the low-fidelity results to the multi-fidelity ones. Since contributions from both fidelities are faithfully taken into account, a robust estimation of the prediction uncertainty of the final multi-fidelity results can be obtained.

This approach is applied here to identify the flame frequency response (FFR). The FFR describes the linear response of a flame to upstream flow perturbations, and

encapsulates the multi-scale multi-physics features of the turbulent combustion dynamics. Additionally, FFR plays a crucial role in the prediction, analysis and control of thermoacoustic instabilities, which are frequently encountered during the operation of low-emission gas turbine combustors.

To thoroughly investigate the effectiveness of the proposed multi-fidelity approach, in the first part of our study, we employ a thermoacoustic network model (a low-order model) where a reference FFR is assumed a priori, to simulate a turbulent swirl premixed burner. This allows us to make systematic assessments of the accuracy, robustness and uncertainty performance of the proposed approach. Two noise levels (high and low) are considered in the current study, and our results indicate that the multi-fidelity approach is particularly preferable in the strong noise case, where a biased and uncertain FFR identified from short-time SI can be effectively corrected by harmonic samples. Thus, this leads to a globally accurate FFR with reduced uncertainty level. We also investigate the sensitivity of the multi-fidelity results to the number and location of frequencies for harmonic excitations, and discuss the optimal strategies for choosing those frequencies.

In the second part of the study, we apply the proposed approach to identify the FFR of a turbulent combustor using signals obtained from large eddy simulations. The identified gain values of the FFR are shown in the figures below. One-third of the computational budget is allocated to perform a short-time SI while the rest is used to perform harmonic excitations. Our multi-fidelity approach aggregates both data and the predicted FFR is more globally accurate and robust, thus demonstrating the effectiveness of the proposed approach.



Future work will focus on developing adaptive sampling schemes to determine the optimal frequencies for harmonic excitations, as well as extending the current multi-fidelity framework to identify frequency responses of other LTI systems.

Numerical modelling of the uncertainties in hip prosthesis material parameters

Fatma ABID[1,2], Abdelkhalak EL HAMI[1], Tarek MERZOUKI[3], Hassen TRABELSI[2], Lassaad WALHA[2], Mohamed HADDAR[2]

[1]Laboratory of Mechanics of Normandy (LMN), National Institute of Applied Sciences of Rouen, Rouen, France

fatma.abid@insa-rouen.fr, abdelkhalak.elhami@insa-rouen.fr

[2] Laboratory of Mechanics, Modeling and Manufacturing (LA2MP), Mechanical Engineering Department, National School of Engineers of Sfax, Sfax, Tunisia

hassen.trabelsi@outlook.fr, walhalassaad@yahoo.fr, mohamed.haddar@enis.rnu.tn

[3]Laboratory of System Engineering of Versailles, University of Versailles Saint Quentin in Yvelines, VELIZY, France

tarek.merzouki@uvsq.fr

The prediction of the mechanical behavior of a bone is a challenging process that has been of agreat attention for reserchers in the biomedical field. The properties of the bone changes from one location to another. Two main types of bone tissue can be distinguished. The inner part is a spongy bone that is characterized by a higher porosity, a higher vascularisation and an ability to absorb energy before the fracture. This type of bone is called cancellous bone. The output bone is characterized by a compact bone. It is called the cortical bone. The composition and the structure of the bone affect its material parameters. However, the composition depends on the nutrition, the disease and the mechanical properties. Kopperdahl and Kevery [1] presented an experimental investigation of the bovine and human specimens. The experiments show that the Young's moduls is related to the bone density. In [2] , the authors study the relationship between the mechanical characteristics and the ash density for the cancellous bone. Kharmanda [3] studied the reliability of a hip prosthesis using a formation material properties. Kharmanda et al. [4] integrate also the multi objactive optimization into an imroved cementless hip prostheis design.

It is worth montioning that the numerical study of such bio mechanical system without taking into account the uncertainties of different parameters has shown a great attention. However, In reality, material parameters show variability and randomness. As a result, the input variation is translated to the output response. Consequently, it is important to carry out an uncertainty analysis that estimates the uncertainty in the hip prosthesis response from the uncertainty in the design variables [5]. In this work, the material parameters are taken as random variables and their influence on the response of the hip prosthysis have been analyzed.

In the literature, we can classify the methods for uncertainty analysis in three main categories: probabilistic methods, non probabilistic methods and analytical methods. Currently, there is a great attention to the probabilistic methods. Among these probabilistic methods, the most frequently used is the Monte Carlo method. This method is widely used due to its robustness and its easy implementation. Nevertheless, the number of achievements must be sufficient. So that, 10^5 or 10^6 deterministic finite element

simulations should be performed to obtain accurate results. The FEM simulation of the hip prosthesis is a complex problem. It takes more time to achieve simulations than a simple problem. Thus, the analysis of the uncertainty using Monte Carlo method will need a large computational time. The spectral stochastic approaches is also a solution for stochastic problem. This method uses a series expansion in order to model a relationship between the uncertainty of the input and thoutput variability. The generalized polynomial chaos (gPC) is considered as one of the spectral stochastic methods. This approach is more efficient to other uncertainties methods. The computational efficiency supplied by the polynomial chaos method is highlited through scientific works in many fields such as solid mechanics [6], fluid dynamics [7] and chemical reactions [8].

The originality of this paper is the increase of the robustness of the hip prosthesis that will operate in presence of uncertainty parameters associated with material properties.

The stochastic approaches described above are coupled with the finite element of hip prosthesis system. A methodology for considering uncertainty in bone materials for a hip prosthesis system is described. The proposed approach is used in order to determine the response of this system with uncertainty related to material parameters. The simulations results are obtained by the generalized polynomial chaos (gPC) method. The proposed technique is an efficient probabilistic tool for uncertainty propagation. It is well shown that the gPC technique is an attractive alternative to the variability studies. For more accuracy, the generalized polynomial chaos results are compared with Monte Carlo simulation.

References

[1] David L Kopperdahl and Tony M Keaveny. Yield strain behavior of trabecular bone. Journal of biomechanics, 31(7):601–608, 1998.

[2] JH Keyak, IY Lee, and HB Skinner. Correlations between orthogonal mechanical properties and density of trabecular bone: use of different densitometric measures. Journal of biomedical materials research, 28(11):1329– 1336, 1994.

[3] G Kharmanda. Reliability analysis for cementless hip prosthesis using a new optimized formulation of yield stress against elasticity modulus relationship. Materials & Design (1980-2015), 65:496–504, 2015.

[4] G Kharmanda. Integration of multi-objective structural optimization into cementless hip prosthesis design: Improved austin-moore model. Computer methods in biomechanics and biomedical engineering, 19(14):1557– 1566, 2016.

[5] Dammak, K., Koubaa, S., El Hami, A., Walha, L., & Haddar, M. (2019). Numerical modelling of vibro-acoustic problem in presence of uncertainty: application to a vehicle cabin. Applied Acoustics, 144, 113-123.

[6] Moez Beyaoui, Manel Tounsi, Kamel Abboudi, Nabih Feki, Lassaad Walha, and Mohamed Haddar. Dynamic behavior of a wind turbine gear system with uncertainties. Comptes Rendus Mecanique 344(6):375–387,2016.

[7] Tonkid Chantrasmi, Alireza Doostan, and Gianluca Iaccarino. Pad´e–legendre approximants for uncertainty analysis with discontinuous response surfaces. Journal of Computational Physics, 228(19):7159–7180, 2009.

[8] Habib N Najm, Bert J Debusschere, Youssef M Marzouk, Steve Widmer, and OP Le Maˆıtre. Uncertainty quantification in chemical systems. International journal for numerical methods in engineering, 80(6-7):789– 814, 2009.

Multi-scale Numerical Simulation of Reinforced Concrete Framed Structure

Tongji University

Prefabricated concrete structures can satisfy the implementation of industrialization and green buildings. Owe to their economic efficiency, less climatic impact, reliable product quality, short construction period and low environmental pollution, prefabricated concrete structures, especially framed structures, have been widely developed in China. The performance of the beam-column joint is the key issue which can affect the seismic performance of the whole structure. Experimental research and multi-scale numerical simulation analysis of cast-in-place frame joints and three kinds of assembled beam-column joints are carried out in this paper.

The experimental study of cast-in-place beam-column joints and three new types of fabricated beam-column joints, which are steel connection joints, sleeve joints and improved steel connection joints, are carried out under low-cycle reversed loading. The comparison of test results shows that the hysteretic curves of steel connection joints is more plump, while possess the best ultimate bearing capacity and energy dissipation capacity.

The shear stress-strain hysteretic relation of cast-in-place beam-column joints was simulated by the micro-scale finite element and the macro-scale element realized by using Joint2D unit in OpenSees while the shear deformation of joint area was considered. The simulated results are in agreement with each other. Due to the complexity of the fabricated steel connection beam-column joints, the micro-scale model will be inefficient to simulate the frame structure design for its complexity. The steel connection joints were simulated by macro-scale joint2D unit to get the shear stress-strain relation skeleton curves while the key parameters such as equivalent elastic modulus of concrete and yield strength of rebar were identified by the two-dimensional space point scatter method which is confirmed by the experimental results.

After that, the cast-in-place frame structure is constituted by the in-suit beam-column joints, and meanwhile, a fabricated frame structure is formed based on the connection manner of the steel connecting joints. . Both of the two frame structures

Formatted: Indent: First line: 0 ch

have six floors and three spans. The reinforcement and dimension of the beam and column for the two framed structures are same, while the joints are different. The whole frame structure is analyzed by the software OpenSees and the joint area was modeled by the macroscopic monolithic joints model. The dynamic time-history analysis of the two frame structures was conducted under the excitation of El Centro wave and the peak acceleration of earthquake motions in elastic and elastic-plastic dynamic time-history analysis is 0.7m/s^2 and 4m/s^2, respectively, which represent the fortification intensity of 8 degrees in China.

For shape steel-connected prefabricated framed structures, the simulated results show that the maximum story drift of the second floor is 4 mm during elastic stage and the inter-story drift ratio is about 1/825. At the elastic-plastic stage, the maximum story drift is 28mm on the first floor, and the inter-story drift ratio is about 1/117. Both the inter-story drifts are smaller than the limit of the inter-story drift at the elastic stage and the elastic-plastic stage, respectively. That meets the design principle of building with no damage under “frequent earthquakes” and no collapse under “major earthquakes”. Therefore, the prefabricated frame structure connected in this way is a feasible connection style. Based on the accuracy of the calculation, the simplified macroscopic joint area model can be used to improve the computational efficiency. This can provide an effective analysis approach for the numerical simulation of the prefabricated framed structures.

Multiscale Moddeling of Self-Affine Rough Contact

A. M. Couto Carneiro[1], R. Pinto Carvalho[1] and F. M. Andrade Pires[1]

[1]Institute of Science and Innovation in Mechanical and Industrial Engineering

{amcc, rcarvalho, fpires}@fe.up.pt

It is well known that, under certain magnification, all surfaces are rough. This has a great impact on many phenomena, such as contact friction, wear, adhesion, thermal behavior and sealing. Moreover, rough surfaces are classified as self-affine, i.e. the roughness features can be observed throughout many scales, down to the nanoscale. The numerical simulation of rough contact, thus, would require prohibitive fine discretization, in order to incorporate all relevant roughness scales.

In this contribution, contact of rough surfaces is analysed using a multiscale finite element framework. Firstly, from a given statistical and spectral surface properties, artificial roughness and profiles are synthesized, by employing a well established non-Gaussian topography generation algorithm [1]. Then, Finite Element meshes are generated from the artificially generated topography, adopting a strategy to reduce, in an orderly fashion, the number of elements with increasing distance to contact regions. Finally, a fully non-linear Finite Element algorithm coupled with a dual mortar contact modelling technique is embedded in a contact homogenization framework [2]. This approach is then used to investigate the effect of the self-affinity of topography on the evolution of the real contact area, comparing the results with analytical models available in literature [3].

[1] Wu, J. J., 2004. Simulation of non-Gaussian surfaces with FFT. Tribology International, 37, 339-349.

[2] Stupkiewicz, S, 2007. Micromechanics of Contact and Interphase Layers. Springer, Verlag Berlin Heidelberg.

[3] Greenwood, J. A. and Williamson, J. P., 1966. Contact of nominally flat surfaces. Proc. R. Soc. Lond. A Math, 295, 300-319.

Presenting Author

Multi-scale adaptive unstructured mesh predictive modelling for environmental problems [1,2,3,4,5]

F. Fang[1*], H. Rong[1], J. Zheng[2], J. Li[3], P. Salinas[1], D. Xiao[4], N.D. Sto. Domingo[5], O. Mark[5], C.C. Pain [1]

[1]Department of Earth Science and Engineering, Imperial College London

[2]Institue of Urban Environment, CAS, China

[3]Institue of Atmospheric Physics, CAS, China

[4]Swansea University

[5]DHI, Denmark

f.fang@imperial.ac.uk

Since multi-physics problems (e.g. coupling of air flow with radiation and chemical reactions for air pollution and atmospheric models) typically have important dynamics that operate over a range of length scales it is necessary to combine these multi-scale methods with multi-physics modeling within the next generation of unstructured mesh models. This provides several profound and widely acknowledged advantages, including: the ability to conform accurately and efficiently to complex domain geometries (for example atomosphere with its geology, an ocean bathymetry or air pollution and flooding a complex cityscape); the ability to dynamically focus resolution and thus focus limited computational resources where it is most required (on areas of particular interest or importance to the dynamics) and simultaneously move the mesh and change the elements/size and shape as well as adapt the order of the accuracy to provide unrivalled numerical resolution/accuracy; and finally, to do all of this in response to the specific modelling needs of the user, while allowing quantitative statements regarding model errors and accuracy to be made. The predictive modelling framework will help determine where discretization and model errors come from and enable us to optimally change our model resolution (e.g. adapt the finite element mesh). The use of adaptive unstructured enables us to resolve physics on a very wide range of spatial scales.

1. Numerical case 1: adaptive mesh modelling in flooding prediction

First, we demonstrate the capability of adaptive meshes in flooding prediction. Over existing adaptive mesh refinement methods (AMR, locally nested static mesh methods),

this adaptive unstructured mesh technique can dynamically modify (both, coarsening and refining the mesh) and adapt the mesh to achieve a desired precision, thus better capturing transient and complex flow dynamics as the flow evolves. Two flooding scenarios are used to assess the performance of a newly developed adaptive mesh flood model (Floodity): the Glasgow's urban flooding event of 2002 and the joint flooding events in Greve, Denmark. The results with use of adaptive meshes have been compared to those from existing models. It has been found that Floodity is able to provide relatively accurate results while the computational cost is reduced by 20 - 88% in comparison to fixed mesh models.

2. Numerical case 2: adaptive mesh modelling in atmospheric and air pollution

Further application of adaptive unstructured mesh is the simulations of air pollution. Once air pollutants are emitted into the atmosphere, the dynamic and chemical processes would transport and transform them continuously. The interactions between these processes involve a wide range of scales. The highly disparate scales pose a formidable challenge for atmospheric and air pollution modelling. In this work, we introduce a new multiscale model for atmospheric and air pollution prediction and controls. The advantage of the adaptive unstructured mesh model has the ability to adapt the mesh according to the evolving pollutant distribution and flow features. That is, the mesh resolution can be adjusted dynamically to simulate the pollutant transport process accurately and effectively. We have successfully applied this new model to a real-life scenario in China – simulated the pollutant released from over 100 coal power plants across 55 cities including Beijing.

3. Machine learning and reduced order modelling

We present new numerical techniques such as, machine learning (ML), reduced order modelling (ROM) and data assimilation (DA), for real-time operational modelling and uncertainty analysis. Having the compatibility of both ML and ROM will be nothing short of revolutionary for a large number of disciplines. Here the capabilities of ML-ROMs have been demonstrated in air pollution, urban flows, ocean, flood prediction. The combination of ROM, ML and DA enables a rapid and accurate modelling response in emergencies.

A Global-Local Zooming Technique

Matthias Birner[1], Marc Alexander Schweitzer

[1]Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI

matthias.birner@scai.fraunhofer.de

In this talk, we present a novel zooming scheme based on global-local enrichments, to tackle multi-site damage problems in laminated composites.

Typically, a classical FEM requ1ires a very large number of degrees of freedom to resolve fine-scale features, as cracks in fracture mechanics problems. Partition of unity methods, as e.g. the GFEM, XFEM or PUM can circumvent this computational overhead by employing problem specific basis functions, so called enrichments. Unfortunately appropriate enrichments are only known analytically or a-priori for a few application cases. Duarte et al. proposed a global-local enrichment method to compute simulation specific enrichments on the fly. Based on this approach we present a zooming scheme that further condenses degrees of freedom and can handle multiple scales present in a problem.

We present numerical results in 2D for laminated composites which show several delamination zones. Here, an essential ingredient is the use of a new set of analytic enrichment functions for bi-material interfaces based on those by Sukumar et al.

C. A. Duarte, D.-J. Kim, and I. Babuška, A global-local approach for the construction of enrichment functions for the generalized fem and its application to three-dimensional cracks, Advances in meshfree techniques, Springer, 2007, pp. 1–26.

N. Sukumar, Z. Y. Huang, J.-H. Prévost, and Z. Suo, Partition of unity enrichment for bimaterial interface cracks, International journal for numerical methods in engineering 59 (2004), no. 8, 1075–1102.

Multiscale prediction of powder properties during pressure-assisted sintering

Szymon Nosewicz [1*], Jerzy Rojek[1], Krzysztof Wawrzyk[1],

Piotr Kowalczyk[1], Grzegorz Maciejewski[2], Marcin Maździarz[1]

[1]Institute of Fundamental Technological Research Polish Academy of Sciences, Warsaw, Poland
[2]Institute of Aviation, Warsaw, Poland
*snosew@ippt.pan.pl

Sintering is a fundamental technology in manufacturing of new advanced materials with many applications, such an automotive or aerospace. Sintering can be defined as the thermal treatment of a powder (or compact) at a temperature below the melting point of the main constituent, for the purpose of increasing its strength by bonding together the particles. The obtained sintered body has a significantly different form compared to the initial state. When powder compacting and sintering occur simultaneously, it is called a pressure-assisted sintering. The evolution of the sintered powder with external pressure is governed by many factors at different scales. Due to the complexity of the process, the description of the sintering phenomenon is a non-trivial task. Macroscopically during sintering, one can observe changes of the bulk material volume (shrinkage) and, associated with this, densification and decrease of porosity. The microstructure during sintering undergoes an evolution characterized by grain rearrangement, increase of grain compaction and formation of cohesive bonds between powder particles which occurs due to mass transport. Surface and grain boundary diffusion are normally dominant mechanisms of mass transport in sintering.

Such a large number of material effects occurring at several scales during sintering cannot be described comprehensively with a single modeling approach. The macroscopic properties are influenced by several factors at various scale interact with one another, hence in numerical modeling we should take into account material phenomena occurring at different levels. In contrast to the traditional approaches, which focus on one scale, multiscale modeling simultaneously considers models at different scales, sharing the efficiency of the macroscopic models as well as the accuracy of the microscopic models.

Such a multiscale approach explores the advantages of lowest scale calculation, for example, molecular simulations, allowing insight into atomic-scale processes at a short time scale, and macroscopic simulations, allowing simulations at a much longer timescale. Constitutive models at various scales are connected which allows us to perform an investigation of various phenomena occurring at different scales.

Within the proposed work, development of numerical models predicting the powder properties during pressure-assisted sintering has been performed for different scales: atomistic, microscopic and macroscopic one. Varied approaches and varied numerical models adequate for each level have been applied. The molecular dynamics (MD) simulations have been performed to determine the diffusive parameters at the atomistic scale. MD simulations allowed to determine the input parameters of micromechanical discrete element model (DEM). By taking into account the composite microstructure, microscopic model has provided data (density and temperature dependent viscosity of material) for macroscopic modeling (finite element framework). The macroscopic constitutive model is based on the assumption that the sintered material is a continuous medium. The numerical model will be validated by the data obtained within the own experimental research by sintering of NiAl powder.

ACKNOWLEDGMENTS

The results presented in the paper have been obtained within the projects funded by the National Science Centre awarded by decision numbers DEC-2013/11/B/ST8/03287.

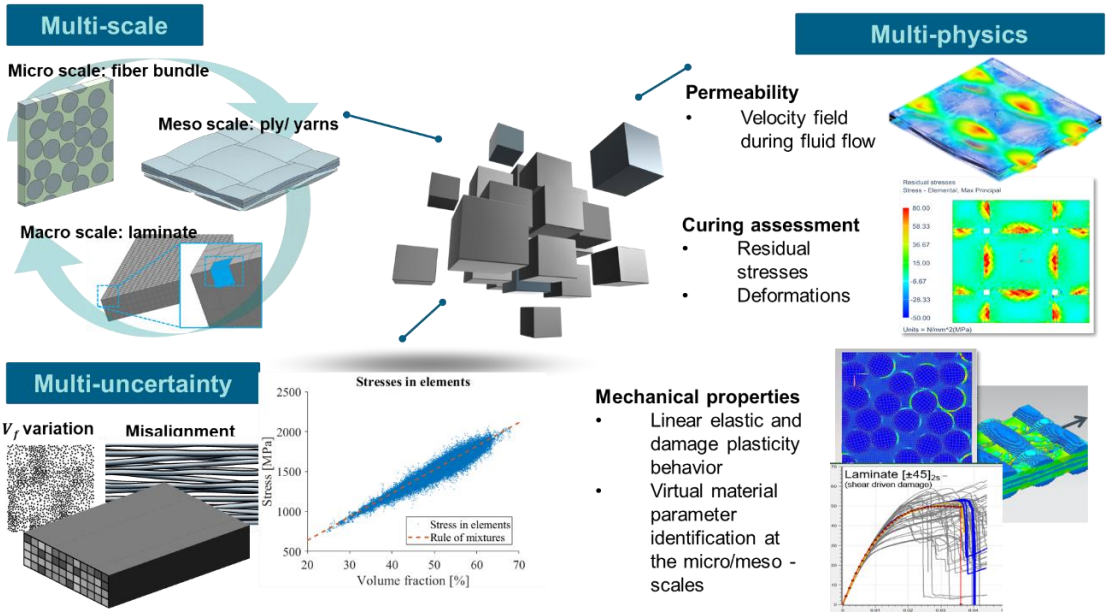
Virtual material characteriazation across scales and physics: case studies

Anna Matveeva, Oxana Shishkina, Fabio Malgioglio, Laszlo Farkas

Siemens Industry Software NV (SISW), Interleuvenlaan 68, 3001 Leuven, Belgium

anna.matveeva@siemens.com

Material engineering for composites is a complex process covering different stages from application-driven design and manufacturing method selection to composite production and performance assessment via iterative optimization loops. Large and expensive test campaign is needed before the final design decision is made. With the Simcenter 3D (Siemens PLM Software) Virtual Material Characterization (VMC), the material engineering process becomes more efficient and can be completed with fewer tests. This contribution demonstrates different stages of a VMC process including solutions for multi-scale, multi-uncertainty and multi-physics problems as depicted in the Figure below.



The modelling workflow of the VMC ToolKit is based on the concept of the representative unit cell (RUC) combined with sequential homogenization schemes for the scale transition. Different material scales and a wide range of supported fiber-reinforced composite types are covered including both, idealized CAD representation and realistic micro-CT-based voxel models.

Three case studies are elaborated in this work. 'The multi-scale' study case focuses on the scale transition for multidirectional laminates. Reverse-engineering of the nonlinear behavior of constituents on the micro-scale is discussed, followed by a virtual parameter identification for the meso-scale ply damage model developed in LMT-Cachan (Ladevèze et al., 1992). 'The multi-physics' cases are linked to the manufacturing simulations. The effect of curing on the development of residual stresses and deformations is studied in thermosetting composite materials on the micro-scale. In order to gain insight into the infusion process, saturated permeability is computed for woven composite RUCs (meso-scale) and first steps towards unsaturated permeability assessment on the micro-scale are discussed. 'The multi-uncertainty' case focuses on the effect of the material variability by the example of a unidirectional composite (UD). The longitudinal tensile strength of a UD ply is predicted, considering the stochasticity of the fiber strength and microstructure (misalignment and fiber volume fraction variability).

The demonstrated Simcenter 3D VMC ToolKit, with a link to micro-CT images, permeability calculations, curing simulations, assessment of the variability and virtual material parameter identification across different material scales, provides an industrial solution for the efficient linking of the manufacturing-induced material features to the materials' performance.

Acknowledgement:

The authors gratefully acknowledge SIM (Strategic Initiative Materials in Flanders) and VLAIO (the Agency Flanders Innovation & Entrepreneurship) for their support of the ICON project M3Strength (Grant no.140158), which is part of the research program MacroModelMat (M3), coordinated by Siemens Industry Software (SISW). O. Shishkina thanks VLAIO for financing her work in the framework of the Innovation Mandate Project "MicroCT-based Model Generation Engine for Virtual Material Characterisation" (Grant no. HBC.2017.0189). F. Malgioglio thanks the EU Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 722626 for funding his work through the FiBreMoD project and his supervisors Prof. S.V. Lomov, Dr. Y. Swolfs, Prof. W. Desmet (KU Leuven, Belgium). The Mechanics of Materials and Structures research group (Ghent University, Belgium) coordinated by Prof. W. Van Paepegem is acknowledged for the support. We thank H. Egami (University of Tokyo, Japan) for his contribution to the research on unsaturated permeability during his internship at SISW through the program "Vulcanus in Europe" by EU-Japan Centre for Industrial Cooperation. We also thank G. Romano (University of Calabria, Italy) for performing study on curing in the scope of the Master thesis internship at SISW.

Heat transfer partitioning models for nucleate boiling

Robin Kamenicky [1], Michael Frank [1], Dimitris Drikakis [2], Konstantinos Ritos [1]

[1]University of Strathclyde, Glasgow, United Kingdom

[2]University of Nicosia, Nicosia, Cyprus

robin.kamenicky@strath.ac.uk

Nucleate boiling is relevant to several industrial sectors, e.g., metallurgy (quenching in manufacturing) and nuclear reactors. Despite considerable efforts [1, 2], the development and validation of nucleate boiling models remains an active field of research.

An essential part of nucleate boiling modeling is the treatment of the (boiling) boundary condition. This paper focuses on heat transfer partitioning models. The efficacy of partitioning models to accurately predict heat transfer depends on the choice of auxiliary models that describe nucleation site density, bubble detachment frequency, and bubble detachment diameter. Various models for specific applications have been proposed [3]. Their applicability depends on the range of pressure, water subcooling, and mass flow rate values. Most of these models were developed for operational conditions in nuclear power reactors. However, there is a number of low pressure, high subcooling applications, such as metallurgical quenching or high power electronics that would benefit from further development.

Although the Kurul & Podowski model [4] is widely used, its robustness and accuracy is questionable. Gilman et al. confirmed the robustness issue, when their numerical prediction suffered from divergence at high heat fluxes [5]. Alternative models have also been proposed [5-7]. Apart from evaporation, quenching and convection heat transfer, the new models account for other heat transfer phenomena such as heat transfer caused by sliding bubbles or the effect of a microlayer. In this paper, various heat transfer partitioning models in conjunction with a conjugate heat transfer boundary condition for the fluid-solid interface, are assessed numerically. The implementation is into the OpenFOAM CFD software. The physics within the solid is modelled using an energy equation, whereas the fluid flow domain is modelled by the Navier-Stokes equations for the vapour and liquid phases.

The models are firstly compared against original experiments used for their development by their authors. This allows to verify proper code implementation. Then the partitioning models are compared using common experiment.

[1] Ilić, M. M., Petrović, M. M., Stevanović, V. D., Boiling Heat Transfer Modelling: A Review and Future Prospectus, Thermal Science, Vol. 23, No. 1, pp. 87-107, (2019).

[2] Chapter 2 - Nucleate Boiling. In: Boiling. Ed. by Yasuo Koizumi et al. Boston: Elsevier, pp. 13–144, (2017).

[3] Cheung, S. C. P., Vahaji, S., Yeoh, G. H., Tu, J. Y., Modeling subcooled flow boiling in vertical channels at low pressures – Part 1: Assessment of empirical correlations, International Journal of Heat and Mass Transfer, pp 736–753, (2014).

[4] Kurul, N., Podowski, M.Z., On the modeling of multidimensional effects in boiling channels, ANS. Proc. National Heat Transfer Con. Minneapolis, Minnesota, USA, pp. 30-40, (1991).

[5] Gilman, L., Baglietto, E., A self-consistent, physics-based boiling heat transfer modeling framework for use in computational fluid dynamics, International Journal of Multiphase Flow, pp 35–53, (2017).

[6] Basu, N. , Gopinath, W., Dhir, V.K., Wall Heat Flux Partitioning During Subcooled Flow Boiling: Part 1—Model Development, Journal of Heat Transfer transactions of The Asme - J HEAT TRANSFER (2005).

[7] Yeoh, G. H., Vahaji, S., Cheung, S. C. P., Tu, J. Y. Modeling subcooled flow boiling in vertical channels at low pressures – Part 2: Evaluation of mechanistic approach, International Journal of Heat and Mass Transfer, pp 754–768, (2014).

A fully coupled electromagnetic-thermal-transient mechanical simulation of the load suffered by aeronautical composite panels during lightning strikes

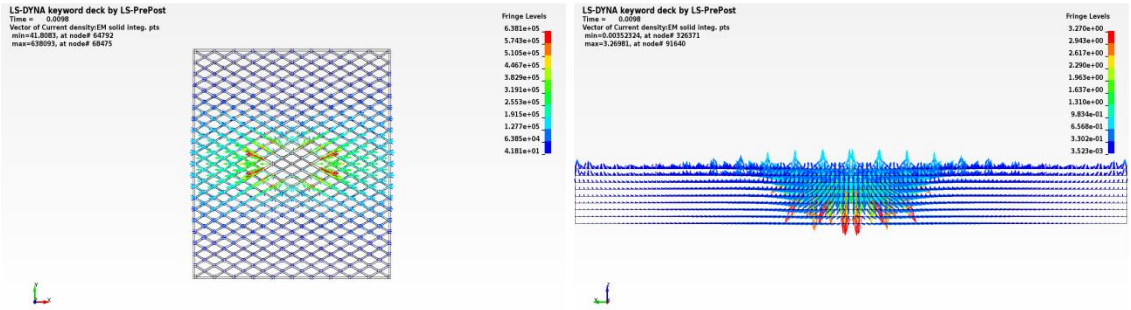
Christine Espinosa [1], Fabio Martarelli [1], Frédéric Lachaud [1]

[1] Institut Clément Ader, Université de Toulouse, ISAE-SUAPERO, IMT MINES ALBI, UTIII, INSA, CNRS, 3 Rue Caroline Aigle, F-31400 Toulouse CEDEX 04, France

christine.espinosa@isae-supaero.fr frederic.lachaud@isae-supaero.fr

One of the main multi-physical and multiscale safety issues facing aircrafts is the protection against lightning strikes. Because of the low electrical conductivity of composites compared to metal, composite aircrafts must be protected against current flows. It is done by metallic mesh coatings. Tests done at AIRBUS showed that when protected by appropriate metallic meshes, composite panels do not delaminate anymore [1]. It has been demonstrated that delamination is mainly due to a resultant mechanical impulse transmitted to the composite panel by the multi-physical phenomena in the protection layers [2, 3, 4]. In presence of paint, the vaporization process is replaced by an explosion which causes delamination [1, 5, 6]. Observed damages in protected GFRP and CFRP or unprotected CFRP panels suggest that the vaporization of the resin of the upper ply of carbon fiber reinforced composite make possible current injection in the composite fibers which causes the explosion [6]. It is thus of primary importance to evaluate the contribution of the different physical components of the lightning strike on the load transmitted to the composite panel, and if the composite is part of its loading.

This talk will present the strategy proposed to model the fully coupled multi-physics behavior of a protected aeronautical panel during the injection of a D-wave current mimicking lightning. A previous coupled FE model allowed us to compute the stress, temperature and current distribution resulting from injection of a D-waveform using a simplified model for the metallic mesh and an evolving injection zone [7]. The predicted mechanical impulse was of the order of magnitude of pressures estimated by energy models [2, 4], but the coarse FE mesh was responsible of oscillations in the Joule resulting temperature and in the pressure. In the present model the FE mesh of the metallic protection is refined and connected to the composite plate through a mechanically thermally and electrically continuous contact. It is shown that current and impulse are indeed the most important load components transmitted to the composite.



Current distribution in the mettalic mesh (left) and the composite panel (right)

[1] A. Bigand, C. Espinosa, J.M. Bauchire, F. Flourens, F. Lachaud (2018). Estimation of the load produced by the electro-thermal behavior of lightning strike protection layers on a composite panel. 18th European Conference on Composite Materials (ECCM18), Athens, Greece.

[2] F. Soulas, C. Espinosa, F. Lachaud, S. Guinard, B. Lepetit, I. Revel, Y. Duval (2018). A method to replace lightning strike tests by ball impacts in the design process of lightweight composite aircraft panels. International Journal of Impact Engineering, 111, 165-176.

[3] A. Bigand, C. Espinosa, H. Rabat, J.M. Bauchire (2018). Lightning strike protection explosion and overpressure profile. 15th High-Technology Plasma Processes (HTPP15), Toulouse, France.

[4] C. Karch, A. Arteiro, P. Camanho (2019). Modelling mechanical lightning loads in carbon fibre-reinforced polymers. International Journal of Solids and Structures, 162, 217-243.

[5] A. Bigand, J.M. Bauchire, C. Espinosa (2018). Lightning arc interaction with complex structure. 15th High-Technology Plasma Processes (HTPP15), Toulouse, France.

[6] A. Bigand, Y. Duval (2017). Quantification of the mechanical impact of lightning strike protection explosion confined by thick paint. International Conference on Lightning and Static Electrocity (ICOLSE), Nagoya, Japan.

[7] C. Espinosa, T. Montel, J. Montes Pons, F. Lachaud, F. Soulas (2017). A numerical study of the pressure applied on CFRP panels during a lightning strike using a coupled electro-thermal-mechanical model. International Conference on Lightning and Static Electrocity (ICOLSE), Nagoya, Japan.

Modelling of shear bands in fluid saturated poroplastic solids with embedded strong discontinuities

Mijo Nikolic[1], Adnan Ibrahimbegovic[2]

[1]University of Split, Faculty of Civil Engineering, Architecture and Geodesy, Split, Croatia

[2]Université de Technologie de Compiègne/Sorbonne Universités, Laboratoire Roberval de Mécanique, Compiègne, France

mijo.nikolic@gradst.hr

Simulations of shear bands require special treatments due to its localized nature. Namely, localized failure is mesh-dependent when standard finite element method is used. Various methods have been developed to tackle this difficulty. However, it is still challenging to be able to simulate this problem in complex environments, such as porous heterogeneous medium with multiple phases and where we could have multiple shear band developments interacting with each other. The presence of fluid inside such medium brings additional complexities. In this work, we present the way to compute such problem in efficient way. The framework for considering multi-phase material with multiple shear bands is based on lattice element method, while pathological mesh dependence with localized failure is eliminated by using embedded strong discontinuities inside elements. No global tracking procedure is required in this approach which also enables easier propagation of multiple bands and their interaction. Moreover, computational algorithms are efficient due to such strategy. Additional strength of the algorithm is that embedded discontinuities are computed at element level and no additional degrees of freedom for existence of localized failure are required. Presence of fluid and its influence to shear band forming is provided with Biot poroelastic approach. Here, we consider material to be plastic with microcracks prior to localized shear band forming. The Darcy law is used to compute fluid flow inside the poroplastic domain.

Acknowledgements: This work has been supported by the Croatian Science Foundation under the project number UIP-2017-05-3429

Comparison of Two New Methods for Fatigue Reliability Analysis

Ruofan Gao[1], Jie Li[2]

[1] School of Civil Engineering, Tongji University, Shanghai, China

gaoruofan529@gmail.com

[2] School of Civil Engineering and the State Key Laboratory on Disaster Reduction in Civil Engineering, Tongji University, Shanghai, China

lijie@tongji.edu.cn

With a review of the previous researches, the traditional fatigue reliability analysis methods are divided into two types, namely, the S-N curve-based methods and the fracture mechanics-based methods. However, both kinds of methods have their limitations. The S-N curve methods lack university, and can hardly indicate the damage development. The fracture mechanics-based models mainly focus on the single macro crack, and cannot reflect fatigue damage state before the formation of the macro crack.

Based on continuous damage mechanics (CDM) and probability density evolution theory (PDEM), this paper develops two new fatigue reliability analysis methods, and compares these two analysis methods from different perspectives. The first new method is based on the remaining fatigue life. Based on the CDM, a stochastic fatigue damage model is introduced for the deterministic structural analysis, by which the fatigue damage process of structure is derived. According to the PDEM, the probability density evolution equation for the remaining fatigue life is built to perform the stochastic analysis. By solving the probability density evolution equation, the probability density function (PDF) of the remaining fatigue life evolving with time is obtained. The fatigue reliability is finally calculated by integrating the PDF of the remaining life. The other new method is the physical synthesis method. The physical equations of solid mechanics are determined by using the stochastic fatigue damage model. Based on the fatigue damage-based failure criterion, the physical synthesis method is developed by combining the physical equations of solid mechanics with the probability density evolution equation. The fatigue reliability is obtained by solving the equations of the physical synthesis method.

The paper compares the theoretical basis of the two new methods for fatigue reliability analysis to illustrate the similarities and differences as well as the advantages

and disadvantages of the two methods. Moreover, the two methods are applied to analyze the fatigue reliability of a concrete continuous beam bridge under random vehicle loading, respectively. The results of fatigue reliability obtained by the two methods are compared in details, to mutually verify the validity of each other and intuitively reflect their advantages and disadvantages.

Construction of optimal basis functions in the Partition of Unity Method and their verification in complex simulations

Denis Düsseldorf [1]

Prof. Dr. Marc Alexander Schweitzer [2]

[1]University of Bonn

[2]University of Bonn and Fraunhofer SCAI

duesseld@ins.uni-bonn.de

In this talk, we present the construction of optimal basis functions for orthotropic laminates with holes that resolve the fine scale details of the solution and the verification of these basis functions in an application setting. The goal of this research is to construct a computational efficient model with very few degrees of freedom, yet approximation properties similar to a fine-scale model so that automatic optimization of layup design and margin of safety assessments including structural details become feasible.

The method is implemented using the Partition of Unity method (PUM), a meshfree generalization of the GFEM or XFEM. The independence of local approximation spaces in the PUM allows us to apply the optimal basis functions in regions where heavy refinement is necessary in the standard methods. We present numerical results in 2D and 3D.

Ivo Babuska and Robert Lipton, Optimal Local Approximation Spaces for Generalized Finite Element Methods with Application to Multiscale Problems, Multiscale Model. Simul., 9(1), 373–406. (34 pages)

A Vibrational study of graphene sheets, carbon nanotubes, and nanocones

Reza Ghaffari [1], Aningi Mokhalingam [2], Shakti S. Gupta [3], Roger A. Sauer [4]

[1,4] Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Templegraben 55, 52056 Aachen, Germany

[2,3] Department of Mechanical Engineering, IIT Kanpur, Kanpur - 208016, India

[1] ghaffari@aices.rwth-aachen.de

[2] aningi@iitk.ac.in

[3] ssgupta@iitk.ac.in

[4] sauer@aices.rwth-aachen.de

In this paper, the frequencies of the transverse vibrations of radially stretched circular graphene sheets, carbon nanotubes, and carbon nanocones are studied comparing atomistic approaches and a new continuum model based on density functional theory data.

The continuum model is nonlinear, hyperelastic, and anisotropic. The strain energy density is written in terms of a set of invariants based on the logarithmic strain and structural tensor [1]. The model is calibrated with density functional theory (DFT) data and implemented in the curvilinear rotation-free finite element formulation of [2]. The employed framework was previously used for the development of membrane and shell material models for graphene [1,3, 4].

In the molecular mechanics simulations, the MM3 potential is used to define the interaction between carbon atoms. The system is first relaxed to the minimum energy configuration. Then, the outer edge atoms are displaced radially untill the required stretch is obtained. The frequencies are found by using the VIBRATE module in Tinker [5].

Molecular dynamics simulations are carried out using REBO+LJ potential in LAMMPS. The minimum energy configuration is equilibrated using a Nose-Hoover thermostat at 0.1 K. Three Nose-Hoover chains are employed to maintain the temperature of the system at the desired level. After pulling the outer edge of the atoms up to a desired stretch, the sheet is deformed into the first mode shape and then allowed to vibrate freely while the total mechanical energy of the system is kept constant. The time history of the

atoms at the center is recorded to calculate the frequencies of vibration using a fast Fourier transform (FFT).

Modal analysis of the circular graphene sheets, carbon nanotubes, and carbon nanocones is conducted using the continuum model and compared with the results from molecular dynamics simulations. The variation of the first frequency versus the surface change J is shown in Fig. (1) for a graphene sheet and the results are in good agreement in all three approaches up to J = 1.2. The deviation of the results is larger for J > 1.2 and - due to the breakage of the bonds for J > 1.4 in Rebo+LJ potential - the results are only presented up to this strain.

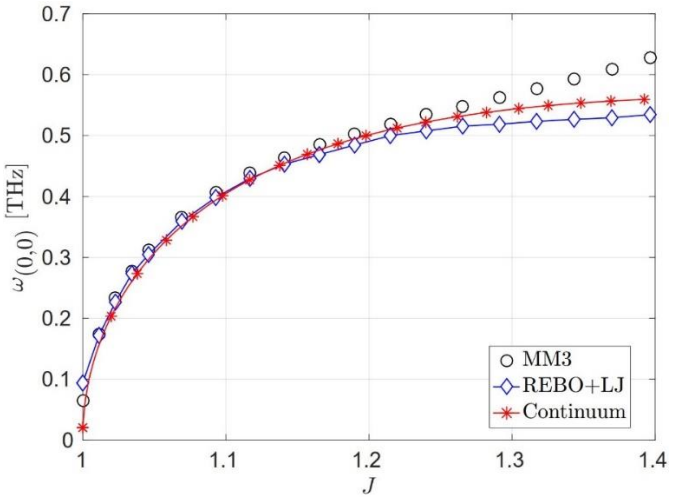


Figure 1: Variation of the first mode frequency versus the surface stretch for a graphene sheet

REFERENCES

[1] Reza Ghaffari and Roger A. Sauer. A new efficient hyperelastic finite element model for graphene and its application to carbon nanotubes and nanocones. Finite Elem. Anal. Des., 146:42-61, 2018.

[2] Thang X. Duong, Farshad Roohbakhshan, and Roger A. Sauer. A new rotation-free isogeometric thin shell formulation and a corresponding continuity constraint for patch boundaries. Comput. Methods in Appl. Mech. Eng., 316(Supplement C):43-83, 2017. Special Issue on Isogeometric Analysis: Progress and Challenges.

[3] Sandeep Kumar and David M. Parks. On the hyperelastic softening and elastic instabilities in graphene. Proc. Royal Soc. Lond. A: Math. Phys. Eng. Sci., 471(2173), 2014. DOI: 10.1098/rspa.2014.0567.

[4] Reza Ghaffari, Thang X. Duong, and Roger A. Sauer. A new shell formulation for graphene structures based on existing ab-initio data. Int. J. Solids Struct., 135:37-60, 2018.

[5] J.W. Ponder. Users guide computer code tinker molecular modelling package 4.2, 2004.

Metamodels for RBDO of wire bonding in microsystem packages

Hamid HAMDANI [1,2] Bouchaïb RADI [2] Abdelkhalak EL HAMI [1]

[1]LMN, Normandie Univ, INSA Rouen, 76000 Rouen, France

[2]LIMII, FST Settat, BP: 577, Route de Casa, Settat, Morocco

hamid.hamdani@insa-rouen.fr, bouchaib.radi@yahoo.fr, Abdelkhalak.elhami@insa-rouen.fr,

For microelectronic device structures, several reliability-based design optimization Methodology (RBDO) was developed. The main objective of such method is to design structures, which should be both economical and reliable where the solution reduces the structural weight in uncritical regions. It does not only provide an improved design, but also a higher level of confidence in the design. This paper focuses on the use of metamodeling technics with high efficiency to overcome the time-consuming of the multiphysics finite element simulation in the RBDO process.

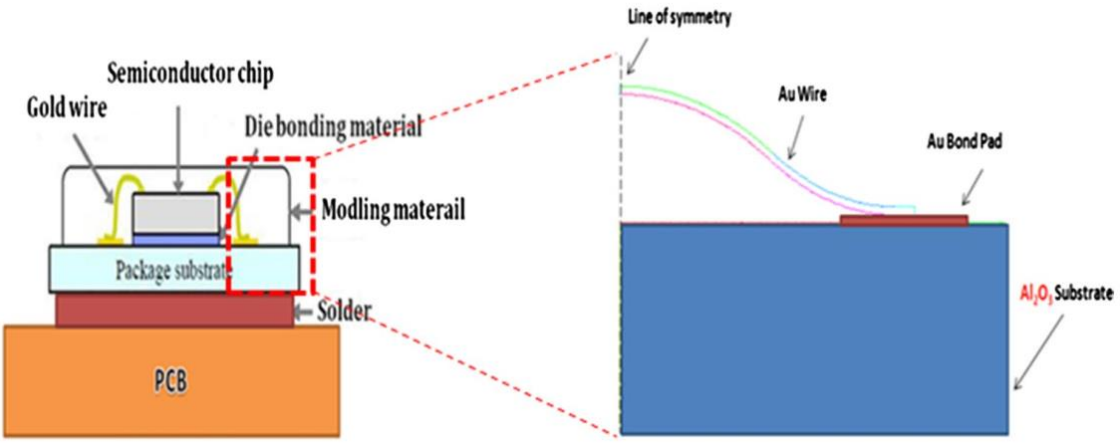


Figure 1: Structure of the electronic package (wire bonding type) and 2D scheme of the model

More precisely, the Finite element simulation model, which intends to analyze the sequence of the failure events in power microelectronic devices, is replaced by appropriate metamodels. The constructed metamodels are validated and compared by cross validation and error measures. Then, the suitable metamodel is chosen according to its quality. The chosen metamodel is used to estimate the probability of failure of power

module. Subsequently the reliability analysis is integrated in the optimization process forming a sequential RBDO algorithm in order to find the best structural designs of wire bonding technologies and to realize the best compromise between cost and safety. The metamodel based RBDO method used in this paper is an approach with high-efficiency and sufficient accuracy. It has improved the traditional methods that use response surfaces without validation.

References

[1] Makhloufi, A., Aoues, Y., and El Hami, A. (2016). Reliability based design optimization of wire bonding in power microelectronic devices. *Microsystem Technologies*, 22(12):2737–2748.

[2] Hamdani, H., Radi, B., and El Hami, A. (2017). Métamodélisation pour une conception robuste des systèmes mécatroniques. *Incertitudes et fiabilité des systèmes multiphysiques*, 2(Numéro 2):10.

[3] Liu DS, Chao YC, Wang CH (2004) Study of wire bonding looping formation in the electronic packaging process using the three-dimensional fnite element method. *Finite Elem Anal Des* 40:263–286

[4] Hamdani, Hamid, Radi, Bouchaïb, and El Hami, Abdelkhalak. Optimization of solder joints in embedded mechatronic systems via kriging-assisted cma-es algorithm. *Int. J. Simul. Multidisci. Des. Optim.* , 10 :A3, 2019.

New Method for Numerical Calibration of a Rotary Kiln Model – A Multiscale Approach

Christian Jordan [1], Mario Pichler [1], Bahram Haddadi [1], Hamidreza Norouzi [2], Florian Wesenauer [1], Jakob Weber [1], Franz Winter [1], Michael Harasek [1]

[1]Institute of Chemical, Environmental and Bioscience Engineering, TU Wien, Getreidemarkt 9/166, 1060 Vienna, Austria

[2]Department of Chemical Engineering, Amirkabir University of Technology, Tehran, Iran

christian.jordan@tuwien.ac.at

Rotary kilns are widely used in industry for the production of a range of products including cement, lime or iron ore pellets and the re-utilization of by-products such as the thermal utilization of solid waste or black liquor in pulp and paper industry. Rotary kilns are also an excellent example of multiple scales: Millimeter sized particles are treated in a device with a characteristic length of several meters.

While there are macroscopic models to describe the global particle movement and filling conditions in a rotary kiln, such as the volumetric fraction of bulk solids, the average residence time or the linear velocity of solids in axial direction, those models provide only a limited amount of information and the validity of the models is typically limited to the calibration space.

For thermal utilization of solid waste not the overall (averaged) residence time, but the residence time of different particle types (material, shape, size) in different zones of the kiln is especially important. Particles are exposed to different conditions (temperatures, gas flow rates, gas composition), along the rotation axis of the kiln - a different combustion and heat- and mass-transfer behavior is expected in each zone.

A detailed simulation of the particle motion in rotary kilns using the Discrete Element Method (DEM) can help to get deep insight in the particle movement and the individual exposure to the kiln environment, the individual residence time profile, as well as particle-particle and particle-wall interactions - however, DEM is computationally expensive. Therefore, DEM simulation data can be used for the calibration of custom-tailored macroscopic models, which are utilized to optimize production processes and equipment in terms of efficiency, product quality and production output and to provide input data for subsequent simulation steps.

In this work experimental investigations and numerical simulations, using the Discrete Element Method, of a lab-scaled rotary kiln have been carried out (see also Figure 1). Focus is the investigation and validation of the residence time of the different particle types in the rotary kiln. The mean residence time and residence time distribution (RTD) in simulation and experiments have been evaluated after reaching a steady state using marked tracer particles. Simulation and experiments show good agreement in terms of mean residence time, RTD and the dynamic angle of repose.

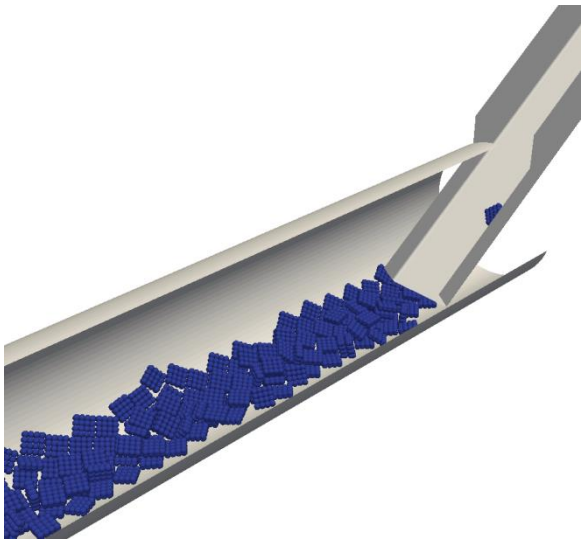


Figure 1 DEM simulation of the lab scale rotary kiln

Using the validated numerical data, the mean residence time profile for each particle type can be calculated for each kiln zone and can then be used for subsequent combustion calculations in 1D or 3D computational fluid dynamics (CFD) models. This combined method is a promising approach for reducing the complexity of the particle movement while keeping relevant information, especially for industrial scaled rotary kilns.

Nanoscience applied to oil and gas technologies: a multiscale computational approach

Caetano R. Miranda [1]

[1]Instituto de Física - Universidade de São Paulo

crmiranda@usp.br

Advances in nanostructured materials have opened a wide range of multifunctional materials with promising potential to control interfaces and flow at nanoscale. Here, I will summarize some of the activities at our group based on multiscale modeling to explore the potential applications of nanoscience for Enhanced Oil Recovery (EOR) processes and fluid flow through nanoporous media. Our strategies are focused on i)Nano-EOR, based on surface drive flow, where mobilisation of hydrocarbons trapped at the pore scale is favored by controlling by the chemical environment through Wetability modifiers and ii)Nano-IOR, through pressure driven flow, by controlling the spatial confinement and fluid flooding at nanoporous. In this hierarchical multiscale protocol, the amount of oil displaced by fluid injection (brine, NP solution, or surfactants) within pore network models (PNMs) is estimated with controlled porosity, size, shape and porous distribution. Initially, the systems of interest are characterized by first principles calculations based on the Density Functional Theory and their atomic interactions validated with interatomic potentials to be used within fully atomistic molecular dynamics (MD)[1-2]. At MD level, the interfacial and transport properties are determined at reservoir conditions. Those properties are mapped into Lattice Boltzmann Method[3] (LBM) parameters to describe the fluid-fluid and fluid-solid interactions. At LBM level, the injection of fluids (brine, NPs and surfactants) is simulated within PNM models previously filled with oil. This can be a useful tool to explore chemical additives for EOR and investigate the wetting effects on fluid behavior and oil displacement in porous media over scales. Applications will be illustrated and the challenges and limitations of this methodology will be discussed.

[1]Miranda et al., Microfluid Nanofluid.,20, 36,2016

[2]Miranda et al., J. Chem. Theory Comput., 14, 3113,2018

[3]Miranda et al., Scientific Rep.,6, 28128,2016

Designing phononic crystal with anticipated band structure through a deep learning based data-driven method

Zhanli Liu [1], Xiang Li [1], Shaowu Ning [1], Zhuo Zhuang [1]

[1] Applied Mechanics Lab., Dept. of Engineering Mechanics, School of Aerospace,

Tsinghua University, Beijing 100084 China

liuzhanli@tsinghua.edu.cn

Phononic crystal is a type of artificial heterogeneous material constituted by a periodic repetition of cells. This characteristic provides a possible solution to the accurate manipulation of acoustic and elastic waves. For this reason, phononic crystal is of application potentials in vibration and noise reduction, filtering, acoustic lens, acoustic imaging, and acoustic stealth, etc. It is thus of significance in the fields of information, communication and medical applications. To design phononic crystal with anticipated manipulation characteristic has become a research hotspot in recent years. However, how to accurately manipulate acoustic and mechanical wave is still a major challenge for existing designing approaches. Assisted by image-based finite element analysis and deep learning, a data-driven approach is proposed in this study for designing phononic crystals. An auto-encoder is trained to extract the topological features from sample images. Finite element analysis is employed to study the frequency bands of samples. A multi-layer perceptron is trained to establish the inherent relation between frequency bands and topological features. The trained models are ultimately employed to design phononic crystals with designated frequency bands. Not limited to this material, the proposed method could be further extended to design various structured mechanical materials with specific functionalities.

Stochastic Finite Element Analysis of U-Shaped RC Shear Wall with a Novel Random Field Modeling Strategy for Open Thin-Walled Structural Members

De-Cheng Feng[1], Yan-Ping Liang[2], Xiaodan Ren[3]

[1]School of Civil Engineering, Southeast University, dcfeng@seu.edu.cn

[2]School of Civil Engineering, Tongji University, 281455107@qq.com

[3]School of Civil Engineering, Tongji University, rxdtj@tongji.edu.cn

The inherent randomness of the material properties, with its coupling with the material nonlinear behaviors, often plays an important role in the analysis and design of structures. Furthermore, some quasi-brittle engineering materials, e.g., concrete, are often inhomogeneous, which means its material properties will vary from point to point within the domain of the structure. To comprehensively represent the mechanical behaviors of structures and elaborately reveal the corresponding damage/failure mechanisms, it is necessary to account for this spatially inhomogeneous effect. Generally, the Stochastic Finite Element Method (SFEM) is adopted to model inhomogeneous structures, in which the material properties are assigned as random fields. Up to date, several celebrated works have been proposed to represent the random field, e.g., spectral representation (SR) method, Karhunen-Loève expansion (KL) method, stochastic harmonic function (SHF) method, etc. However, most of the existing strategies are developed for the modeling of random fields spanning on the Euclidean space, e.g., a 2D plane space, while it remains a challenge for the definition of the random fields on manifolds and curved surfaces.

In the present work, a novel random field modeling strategy for open thin-walled structural members is developed. The manifold occupied by the open-thin walled structural member is mapped to the 2-D Euclidean space using the manifold learning methods, then the well-known random field representation methods can be directly employed. Theoretically, either SR, KL and SHF methods can be adopted. Nevertheless, considering the balance between numerical accuracy and computational efficiency, the SHF method is used herein due to the reduced number of basic random variables. The above mentioned strategy is then integrated with the softened damage-plasticity model, which can accurately reproduce the typical nonlinear behavior of quasi-brittle materials, to perform the stochastic finite element analysis. Moreover, the probability density

evolution method (PDEM) is also introduced to obtain the instantaneous probability density function of the structural responses through the results by SFEM. Finally, the proposed framework is applied to the analysis of U-shaped reinforced concrete shear walls, and the stochastic behaviors, e.g., bearing capacity, energy dissipation and damage evolution, are obtained and discussed.

Increased Modelling Demands by Moving from Resolved to Unresolved Simulation of Heterogeneous Reactive Systems

Bahram Haddadi[1], Christian Jordan[1], Michael Harasek [1]

[1]Technische Universität Wien, ICEBE

bahram.haddadi.sisakht@tuwien.ac.at

Catalysts can be used for speeding up reactions. For a certain catalytic reaction, the surface area of the catalyst available to the reactants plays an important role in the performance of the processes. Packed beds are a robust solution for increasing the surface area between fluid and solid because of their stable and economic operation. The catalytic reaction behavior in the packed can be investigated whether experimentally or using simulation approaches. Although experiments can provide valuable information about the system, they are time consuming and costly. On the other hand, verified simulation approaches can provide detailed information about the processes in a reasonable cost.

Among available simulation approaches, computational fluid dynamics (CFD) is a valuable tool for investigating mentioned heterogeneous systems, since it can provide time and space resolved information. The main reason that lagged CFD in this field behind compared to the other simulation methods is the very high computational overhead for simulating these systems in fully resolved mode – resolving the geometry of each particle. This drawback can be overcame by simulating packed beds using an unresolved approach. In the unresolved approach, particles are not resolved but models are used for describing their effect on the flow and reaction behavior. For choosing the appropriate models, the main point is the capability of the chosen models on representation of the local and global phenomena.

In this study, the effect of different void fraction (porosity) models on unresolved simulation of a catalytic reaction in a packed bed was investigated. Dehydrogenation of n-octyl alcohol (octanol) over Cu^0 catalyst was simulated in a packed bed with bed/particle ratio of approximately eight. The simulated bed was filled up to 200 mm, octanol vapor was entering from bottom of the bed, and the products were exiting from the top. As a reference, the resolved bed was simulated using the suggested reaction kinetics and equilibrium in the literature [1]. For simulating the bed using unresolved

approach two models were used for porosity changes along bed radius: constant porosity and a porosity profile using the de-Klerk correlation. The overall conversion at the end of the column is similar for all three beds. The radial distribution of the octanol concentration can be found in Figure 1. As it can be seen, using more accurate physical model (de-Klerk) represents the local phenomena better compared to the other global model.

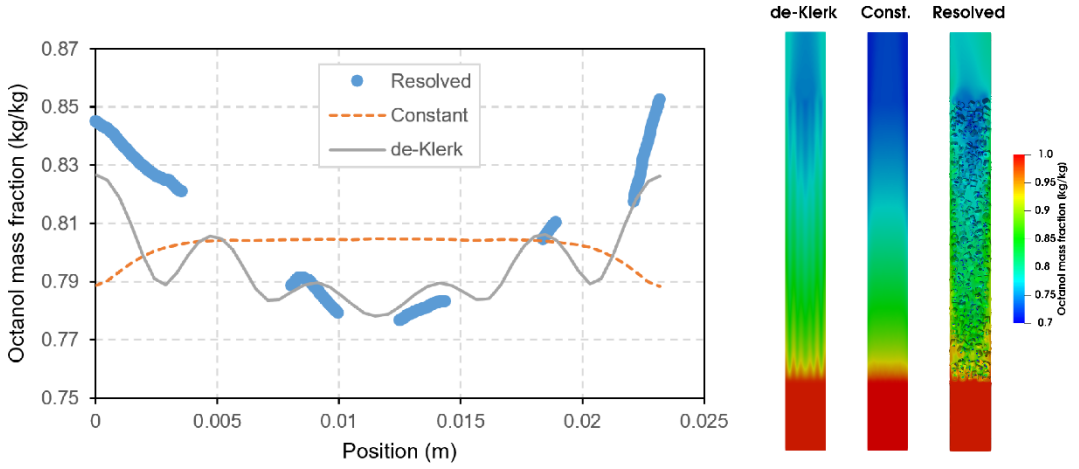


Figure 1. Octanol concentration at 0.1 m from bottom of a reactive catalytic packed bed. Resolved: catalytic particles surfaces are fully resolved – the local gaps in the graph show the particles positions, Constant: a constant radial porosity was used for unresolved modeling, de-Klerk: the radial porosity was modeled using de-Klerk correlation [2]

[1] M. E. Crivello, C. F. Pérez, S. N. Mendieta, S. G. Casuscelli, G. A. Eimer, V. R. El'\ias, and E. R. Herrero, "n-Octyl alcohol dehydrogenation over copper catalysts," *Catal. Today*, vol. 133, pp. 787–792, 2008.

[2] A. De Klerk, "Voidage variation in packed beds at small column to particle diameter ratio," *AIChE J.*, vol. 49, no. 8, pp. 2022–2029, 2003.

A Turbulence Based Sensitivity Study on Drag Prediction of the NASA Common Research Model Aircraft

Şule Öztürk [1], Berkay Pirlepeli[1], Mehmet Yılmaztürk[1] & Melike Nikbay[1]

[1]Istanbul Technical University

ozturksu15@itu.edu.tr, pirlepeli18@itu.edu.tr, yilmazturkm@itu.edu.tr, nikbay@itu.edu.tr

A great amount of effort has been spent several years to obtain the accurate numerical solution of flow over transonic commercial aircrafts and other aerospace industries by using the tools of Computational Fluid Dynamics (CFD). Estimation of the proper drag coefficient has been the most challenging with compared to the all other aerodynamic coefficients. There is a great deal of works to develop the CFD tools namely the geometry modeling, grid generation, numerical algorithms and turbulence modeling to get the proper and efficient solution of Reynolds-Averaged Navier-Stokes (RANS) equations for the flow field of complete aircraft configurations. One of the most important of these studies is the drag prediction workshops focused on the Common Research Model (CRM) Aircraft organized by National Aeronautics and Space Administration (NASA). [1]

The purpose of this study is to examine the structural and aerodynamic characteristics also the sensitivities of the turbulence model closure constants on the aerodynamic coefficients of NASA's CRM. For this purpose, Fluid Structure Interaction (FSI) and the CFD simulations will be performed on the Wing-Body-Tail (WBT) geometry using a commercial (FLUENT) software and an open source (SU2) software. Assuming the given reference flow conditions, the analyzes were carried out at different angle of attacks. The RANS equations were solved with Spalart-Allmaras(SA) and Menter's SST k-ω (SST) turbulence models. To verify the fidelity of simulations, the results will be compared with experimental and other study results. Finally, to determine the effect of SA and SST closure constants on the aerodynamic coefficients, a sensitivity study will be performed using Sobol indices and the optimal values for the turbulence model parameters will be determined. During studies all the necessary data and geometries are received from NASA. [2]

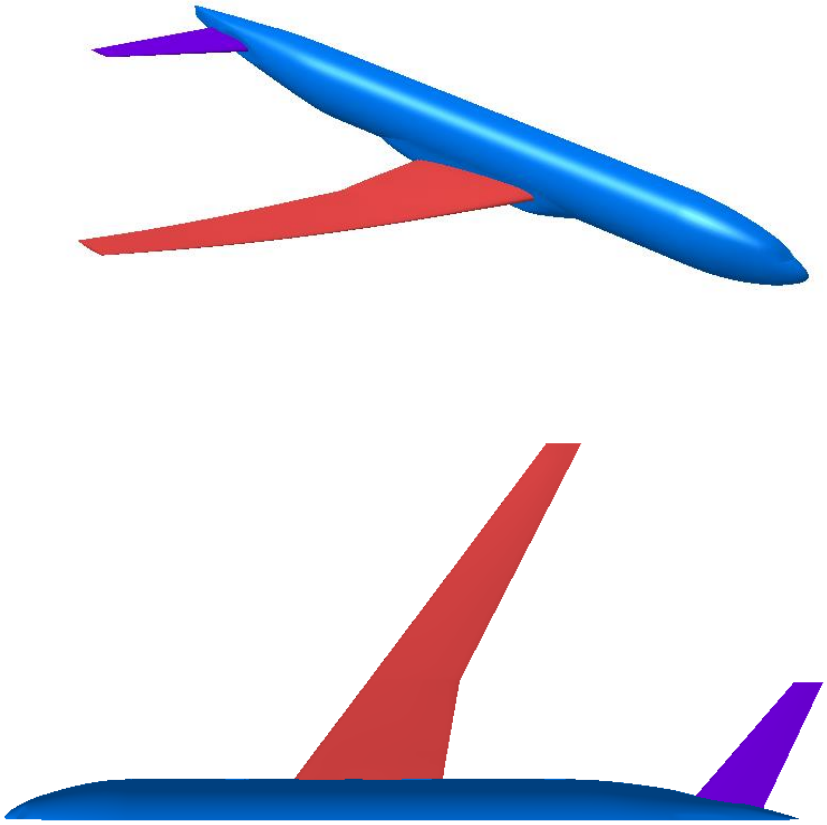


Figure 1 NASA CRM Aircraft WBT Geometries [2]

REFERENCES

[1] *6th AIAA CFD Drag Prediction Workshop* Retrieved April 14, 2019, from https://aiaa-dpw.larc.nasa.gov/

[2] *NASA Common Research Model* Retrieved April 14, 2019, from https://commonresearchmodel.larc.nasa.gov/2012/01/19/hello-world-2/

Approximation of frequency response functions with the multi-element generalised polynomial chaos method

Prem Ratan Mohan Ram [1], Ulrich Römer [1]

[1]Institut für Dynamik und Schwingungen, Technische Universität Braunschweig

p.mohan-ram@tu-bs.de

While designing or analyzing engineering systems, it is often the case that one is interested in analysing the effects of input uncertainties on response functions in the frequency domain. In cases where such a response is computationally expensive to compute, it becomes particularly necessary to compute a cheap surrogate model for uncertainty quantification purposes. It is also desired that such a surrogate is able to approximate the response accurately throughout the operating frequency range.

In many cases, while dealing with acoustic or electromagnetic systems for instance, this is quite challenging as it is common for these systems to exhibit sharp variations in their response for small changes in frequency. Lately two approaches, namely the Padé approximation technique and the polynomial chaos method are receiving increasing interest in this context. A general formulation of Padé-type approximations for multi-variate problems is still a work-in-progress [1]. The polynomial chaos method, on the other hand, requires a very high polynomial order to accurately approximate such response functions. Instead of using a high polynomial order on a global polynomial chaos expansion (GPCE) for the entire parameter domain, in [2], the multi-element generalized polynomial chaos expansion (MEGPCE) method has been proposed, which adaptively decomposes the domain of the random parameters into sub-domains, for each of which a local polynomial chaos expansion is computed. This allows using smaller elements at areas where the response varies sharply and larger elements elsewhere, thus performing a piecewise polynomial approximation.

In this work, we analyse the use of the MEGPCE to approximate frequency response functions which depend on random model parameters. Special emphasis is put on suitable error estimation techniques, which are required for adaptivity. In the original work [2] a variance-based criterion for adaptivity was proposed, which is easily computable in a polynomial chaos context. As pointed out in [3], using the relative

variance error as an indicator involves comparing this error against a free parameter, which lacks a physical meaning, to decide whether a particular element has to be further divided or not. In [3], this problem of fixing a free parameter is avoided by using the residual error, computed by using the approximated solution in the governing system of equations, to steer the MEGPCE algorithm. We additionally investigate the use of an adjoint error indicator [4] in the MEGPCE, which indicates the error in approximating the actual quantity of interest. Such an error indicator, being goal-oriented, promises quick convergence to the required quantity of interest.

We apply the MEGPCE to approximate frequency response functions of systems of the form

$$(-\omega^2 M + i\omega C + K)X = F \qquad (1)$$

, where the mass (M), damping (C) and stiffness matrix (K) may contain random input parameters. The behavior of several mechanical and electronic systems can be modelled with (1). We give several numerical examples and analyse the convergence of the MEGPCE method in approximating frequency response functions. Moreover, we assess and report on the efficiency of different error criteria mentioned above.

References:

[1] T. Chantrasmi, A. Doostan, G. Iaccarino, Padé–Legendre approximants for uncertainty analysis with discontinuous response surfaces, Journal of Computational Physics 228 (2009) 7159–7180

[2] X. Wan, G. E. Karniadakis, An adaptive multi-element generalized polynomial chaos method for stochastic differential equations, Journal of Computational Physics 209 (2005) 617–642

[3] B. Chouvion, E. Sarrouy, Development of error criteria for adaptive multi-element polynomial chaos approaches, Journal of Mechanical Systems and Signal Processing 66, DOI: 10.1016/j.ymssp.2015.05.007

[4] T. Butler, P. Constantine, T. Wildey, A posteriori error analysis of parameterized linear systems using spectral methods, SIAM J. Matrix Anal. Appl. 33 (2012) 195–209

Optimization of Control Parameters for an Electrified Vertical Take-off Landing Vehicle Using the Integral Squared Method

Ibrahim Cicek [1] and Prof. Dr. Melike Nikbay[2]

Istanbul Technical University

cicekib@itu.edu.tr

nikbay@itu.edu.tr

Electrified vertical take-off and landing (EVTOL) aircrafts are studied on contemporarily for their robust maneuvers and cost efficient flight operations. By mounting electric propulsion systems, EVTOLs are considered clean vehicle for next generation air transportation. To optimize flight performance of an EVTOL by minimizing power consumption and maintaining smooth maneuvers, the sought after values of control parameters are computed using the optimal control theory. System is to be modeled as closed loop linear control system with calibretable parameters. The aim is to tune control parameters sequentially by determining desired performance output resulting from the sequential inputs.

In this paper, a study on optimization of electrified vertical take-off landing aircraft control parameters is achieved by eliminating Integral Squared Errors - ISE method using the optimal control theory. Literally, error to be eliminated is discrepancy between target reference and actual state of flight maneuvers, when actuator inputs and systems response mismatch. In this case, the employed performance parameters are rise time, settling time and percentage overshoot of vehicle states over a specified time interval. These parameters are input for performance measure function which is objective function of the problem. System constraints are predefined for vehicle flight comfort and implemented into the Lagrange Multiplier Method for constrained non-linear optimization. Moreover, the method of eliminating steady state error is described by Parseval's Theorem for linear control systems.

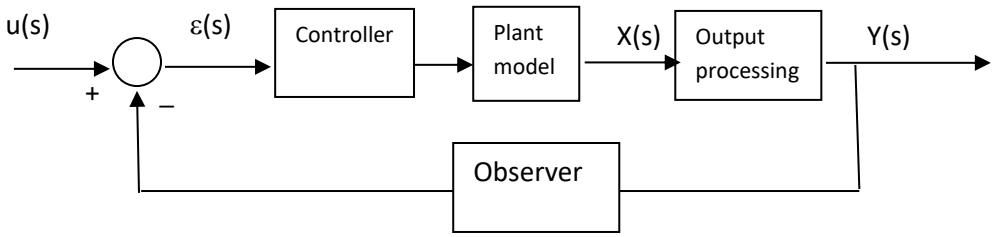


Fig1. Optimized system control scheme

The problem is modeled by mathematical representation of optimization probles as shown below with integral squared error measure J and predefined constraint C, eq(1) and eq(2). Parameters which related performance measure are are a, b, n ,m constants and calculation is done within time interval of [t=0, t_f] . Here t_f is arbitrary.

Minimize the defined performance index ;

$$J^* = \int_0^{t_f} \varepsilon(t)^2 dt$$

Subject to performance measure of;

$$C = \int_0^{t_f} a[X(t)^n \pm bY(t)^m]dt$$

Where C is constrained between limits of –k < C < +k.

References

[1] D.E. Kirk, *Optimal Control Theory An Introduction*, 1970, Prentice Hall, New Jersey.

[2] M. Nikowitz, *Advanced Hybrid and Electric Vehicles System Optimization and Vehicle Integration*, 2016, Springer, Vienna Austria.

[3] Y.S. Wang, *A System Level Approach to Optimal Controller Design for Large-Scale Distributed Systems, 2017*, California Institute of Technology.

[4] Y.L. Leong, *Optimal Controller Synthesis for Nonlinear Systems, 2017*, California Institute of Technology.

Assessment of the Size of the Representative Volume Element of Random Heterogeneous Materials

Paweł Hołobut [1]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences

pholob@ippt.pan.pl

One of the main concepts in micromechanics of materials and homogenization theory is the Representative Volume Element (RVE). There exist several imprecise definitions of the RVE, describing in qualitative terms a similar entity. The RVE is generally understood as a cubic volume of material which is macroscopically small, but simultaneously large enough to well represent the material's microstructural features in the statistical sense. In particular, the RVE's overall physical properties should be effective in the sense of being invariant with respect to choosing a different sample or further increasing the size of the cube. The RVE size depends on the physical property being considered (elastic or plastic properties, thermal conductivity, etc.), geometry of the microstructure (number of phases and their spatial arrangement), and the differences between the properties of individual phases [1]. The RVE is generally assumed to be large compared with the size of inhomogeneities; however, effective properties can sometimes be estimated using cubes of relatively small sizes [2].

In periodic materials, the RVE can be selected as the elementary periodic cell. In heterogeneous materials with random morphology, however, determination of the size of the RVE is not straightforward. Due to random spatial variations of the microstructure, two samples of the same random material may differ in their average response beyond an acceptable tolerance limit. This problem is frequently investigated using the notion of the Stochastic Volume Element (SVE) [3]. The SVE is a mesoscale volume element, whose size varies between the average size of inhomogeneities and the size of the RVE. The overall properties of the SVE, called apparent properties, are functionals over random fields describing the microstructure and may have significantly different values for different samples. As the size of the SVE increases, more and more inhomogeneities tend to be enclosed in the cube and the laws of large numbers cause that apparent properties tend to effective ones with increasing certainty. In this way, the SVE approaches the RVE.

The present work is devoted to probabilistic analysis of the size of the cube at which the transition from the SVE to the RVE can be assumed to occur. An attempt will be made to provide a precise, quantitative stochastic definition of the RVE, denoting an SVE of such dimensions that the probability of obtaining two samples with apparent properties differing by more than a given error threshold is sufficiently small. This is a slight modification and formalization of the approach proposed in [1]. Fundamental stochastic characteristics such as mean values and covariance matrices of apparent mechanical properties of SVEs will be presented for several example morphologies. Using the proposed definition of the RVE and the computed stochastic characteristics, approximate RVE sizes will be obtained and validated against results of numerical homogenization.

References

[1] T. Kanit, S. Forest, I. Galliet, V. Mounoury, D. Jeulin. *Determination of the size of the representative volume element for random composites: statistical and numerical approach*. International Journal of Solids and Structures, Vol. 40, pp. 3647–3679, 2003.

[2] A. El Moumen, T. Kanit, A. Imad, H. El Minor. *Effect of reinforcement shape on physical properties and representative volume element of particles-reinforced composites: Statistical and numerical approaches*. Mechanics of Materials, Vol. 83, pp. 1–16, 2015.

[3] M. Ostoja-Starzewski. *Material spatial randomness: From statistical to representative volume element*. Probabilistic Engineering Mechanics, Vol. 21, pp. 112–132, 2006.

Scaling procedure for the design of a validation experiment on an accidental gas release

Anna Chiara Uggenti[1], Alberto Moscatello[1], Gaetano Iuso[1], Domenic D'Ambrosio[1], Gioacchino Cafiero[1], Raffaella Gerboni[1], Andrea Carpignano[1]

[1]Politecnico di Torino, Corso Duca degli Abruzzi, 24, Torino, Italy

anna.uggenti@polito.it, alberto.moscatello@polito.it, gaetano.iuso@polito.it, domenic.dambrosio@polito.it, gioacchino.cafiero@polito.it, raffaella.gerboni@polito.it, andrea.carpignano@polito.it

Oil&Gas platforms are complex structures characterized by the presence of flammable and pressurized fluids and by a unique working environment, with limited spaces and congested presence of processing equipment. Risk assessment on these structures is mandatory according to international directives and it involves the evaluation of frequencies and consequences of possible accidental scenarios.

The Italian Ministry of Economic Development is supporting the SEADOG (Safety and Environmental Analysis Division for Oil&Gas) laboratory at Politecnico di Torino to develop research projects on Oil&Gas offshore safety. At SEADOG, we have developed an innovative CFD hybrid approach to simulate the consequences of accidental gas releases.

This approach simulates two separate and consequent steps that happen in an accidental gas jet release: the first one is the initial supersonic behavior modeled into a portion of the total platform domain; the second step is the following subsonic dispersion of the released gas into the total domain. The supersonic characteristics appear within the first tens of centimeters from the release point, where the compressibility effects drive the phenomena evolution. The subsonic dispersion domain may corresponds to entire platform (tens of meters), where the fluid can be treated as incompressible. The two steps are computationally evaluated and optimized separately, while the coupling follows.

A key boundary condition for the phenomenon simulation is the wind speed. This real scale speed has to be defined according with the typical velocity distribution of the atmospheric wind present in the location (Adriatic Sea) where the platform is positioned.

To validate this theoretical approach, a physical experiment is designed for the investigation in a wind tunnel of a scaled (1:10) mockup of a real platform will be equipped with a gas release supply line and a sensors' network.

While the mock up is scaled according to a geometric ratio, a finer assessment is needed to apply the correct scaling approach to define the reference speed in the wind tunnel and the mass flow release.

The scaling of the wind velocity has followed the scaling theory for wind tunnels, respecting the logarithmic evolution of the wind profile in proximity to the sea surface.

The scaling of the mass flow release is inspired by the approach proposed by Hall and Walker (1997) with some adjustments to fit our specific case.

In particular, a dimensionless group is chosen to link pressure release, nozzle diameter, scaling factor and gas properties: the dimensionless discharge momentum flux. Furthermore, this group contains information about both the real and the scaled wind velocity.

The approach proposed in this paper aims at scaling supersonic jet releases, maintaining their critical behavior for the test.

A selection of case studies will be tested in the experimental setup to be built by the end of year 2019 under the supervision of the SEADOG research team.

Reference

Hall D. J. and Walker S., "Scaling rules for reduced-scale field releases of hydrogen fluoride", Journal of Hazardous Materials, vol. 54, pp. 89-111 (1997)

A DFT study of single layer blue phosphorus and its implementation in a continuum model

Farzad Shirazian [1], Reza Ghaffari [2], Ming Hu [3], Roger A. Sauer [4]

[1,2,4] Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Templegraben 55, 52056 Aachen, Germany

[3] Department of Mechanical Engineering, University of South Carolina, 541 Main Street, Columbia, SC 29208, USA

[1] shirazian@aices.rwth-aachen.de

[2] ghaffari@aices.rwth-aachen.de

[3] hu@sc.edu

[4] sauer@aices.rwth-aachen.de

The mechanical properties of single layer blue phosphorus are studied using density functional theory (DFT). The simulations are carried out using the Quantum Espresso package [1]. An ultrasoft pseudopotential and the Perdew-Burke-Ernzerhof (PBE) exchange correlation functional are used in the DFT simulations. The considered unit cell is periodic and consists of two phosphorus atoms. In order to eliminate the interaction with replicates in the out-of-plane direction, a vacuum space has been considered in the unit cell.

First, the atomic structure of blue phosphorus is obtained. The lattice parameter is 3.28 Å, the thickness of the monolayer is 1.23 Å, and the length of the P-P bond is 2.26 Å. Then, an optimal set of virtual tests is designed to obtain the mechanical behavior of blue phosphorus. Two uniaxial stretches along the zigzag and armchair directions and one pure dilatation virtual test are chosen, and the strain energies and stresses are calculated for various strains. At each step, the strain is applied to the boundary of the unit cell and the atoms are relaxed while keeping the unit cell fixed.

The generated data are then used to calibrate a nonlinear, hyperelastic, and anisotropic continuum model that is then implemented in the curvilinear rotation-free finite shell element formulation of [2]. The employed framework has been previously used for the development of membrane and shell material models for graphene [3, 4, 5].

The model is then used to simulate the micro-indentation of single layer blue phosphorus as an example.

In order to validate the model and show its ability to capture anisotropic behavior of single layer blue phosphorus, the virtual uniaxial stretch test is conducted in other directions. The results are presented in Fig. (1). The continuum model shows good agreement with DFT calculations. More results are available in [6].

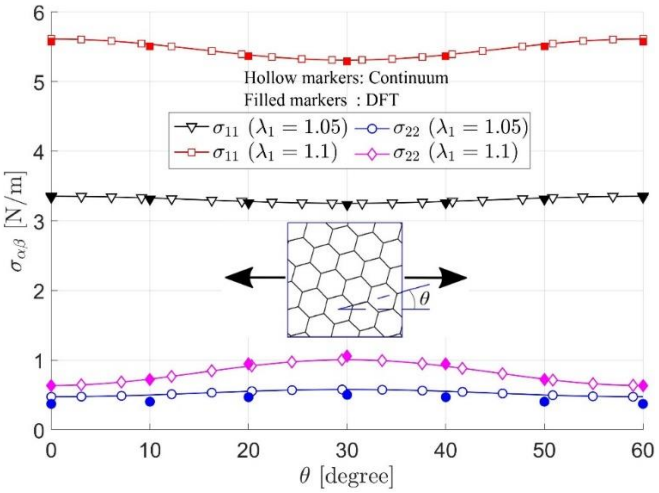


Figure 1: Comparison of the DFT and continuum results for stress σ_{11} and σ_{22} for a stretch in direction θ with respect to the armchair direction. The figure is taken from [6].

REFERENCES

[1] P. Giannozzi et. al. Quantum espresso: a modular and open-source software project for quantum simulations of materials. J. Phys. Condens. Matter, 21(39):395502, 2009.

[2] Thang X. Duong, Farshad Roohbakhshan, and Roger A. Sauer. A new rotation-free isogeometric thin shell formulation and a corresponding continuity constraint for patch boundaries. Comput. Methods in Appl. Mech. Eng., 316(Supplement C):43-83, 2017. Special Issue on Isogeometric Analysis: Progress and Challenges.

[3] Sandeep Kumar and David M. Parks. On the hyperelastic softening and elastic instabilities in graphene. Proc. Royal Soc. Lond. A: Math. Phys. Eng. Sci., 471(2173), 2014. DOI: 10.1098/rspa.2014.0567.

[4] Reza Ghaffari, Thang X. Duong, and Roger A. Sauer. A new shell formulation for graphene structures based on existing ab-initio data. Int. J. Solids Struct., 135:37-60, 2018.

[5] Reza Ghaffari and Roger A. Sauer. A new efficient hyperelastic finite element model for graphene and its application to carbon nanotubes and nanocones. Finite Elem. Anal. Des., 146:42-61, 2018.

[6] Reza Ghaffari, Farzad Shirazian, Ming Hu, and Roger A. Sauer. A nonlinear hyperelasticity model for single layer blue phosphorus based on ab-initio calculations. arXiv e-prints, page arXiv:1902.05128, Feb 2019.

A Fully Second-Order Homogenisation Model for the Analysis of Multi-Phase Materials at Finite Strains

Igor A. Rodrigues Lopes [1], Francisco M. Andrade Pires [2]

[1,2] Faculty of Engineering of the University of Porto, INEGI

[1] ilopes@fe.up.pt, [2] fpires@fe.up.pt

Multi-scale analyses are of utmost importance in order to understand the micro-scale mechanisms that influence the macroscopic material behaviour. Materials which are heterogeneous at a certain spatial scale may be modelled by a Representative Volume Element (RVE), where phenomena arising at the micro-scale due to a macro-scale loading may be analysed in detail, accounting for the effect of material heterogeneities.

Second-order homogenisation-based multi-scale models where the macro-scale is modelled as a second-order continuum, while the micro-scale is described by the classical first-order continuum mechanics [1,2,3], enable the modelling of moderately high strain gradients at the macro-scale and allow the analysis of deformation modes like bending or torsion at the micro-scale. In addition, the homogenised response is influenced by the RVE length, that acts as a length-scale parameter in the macro-scale constitutive response. Nevertheless, this kind of models is not able to capture size effects due to the length of the micro-constituents.

In the present contribution, a fully second-order homogenisation model, where the material behaviour is modelled with a second-order continuum at both scales, is formulated. Due to the characteristic length introduced at the micro-scale through the second-order constitutive equations, the influence of the constituents' size is included in the model. The numerical solution of the resulting micro-macro coupled problem is described in detail with mixed finite elements. Illustrative examples are employed to show the capabilities of the presented model to describe distinct aspects of the material behaviour at both scales.

REFERENCES

1. V.G. Kouznetsova, M.G.D. Geers and W.A.M. Brekelmans, Multi-scale constitutive modelling of heterogeneous materials with a gradient-enhanced computational homogenization scheme. *Int. J. Numer. Meth. Eng.*, Vol. **54**, pp. 1235-1260, 2002.

2. D.J. Luscher, D.L. McDowell and C.A. Bronkhorst, A second gradient theoretical framework for hierarchical multiscale modeling of materials. *Int. J. Plast.*, Vol. **26**, pp. 1248-1275, 2010.
3. P.J. Blanco, P.J. Sánchez, E.A. de Souza Neto and R.A. Feijóo, The method of multiscale virtual power for the derivation of a second order mechanical model. *Mechanics of Materials*, Vol. **99**, pp. 53–67, 2016.

Ductile failure analysis in metallic materials through computational homogenisation

R. P. Cardoso Coelho [1], D. de Bortoli [1], R. Pinto Carvalho [1], F. M. Andrade Pires [1]

[1]Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI), Faculty of Engineering, University of Porto

{ruicoelho,ddbortoli,rcarvalho,fpires}@fe.up.pt

The ductile failure of metals at low homologous temperatures is largely determined by the nucleation, growth and coalescence of microstructural voids. These phenomena are strongly dependent on the stress state, specifically on parameters such as triaxiality and Lode angle. High triaxiality stress states tend to increase the void size, whereas lower triaxialities distort them significantly. The Lode angle has a smaller but still noticeable effect on ductile failure. Over the last years, the modeling of heterogeneous materials by an interchange of information between the macro and micro scales has received increasing attention, especially by the analysis of microscopic Representative Volume Elements (RVEs) and the homogenization of its response to obtaining its macroscopic counterpart[1,2].

The main purpose of this contribution is to investigate the influence of factors such as loading path, material properties and void geometry on the overall macroscopic response. Using the finite element method, several RVEs containing voids are analyzed, subjected to different boundary conditions, with both isotropic (von Mises) and anisotropic (mono- and polycrystalline FCC and BCC slip) matrix material models. A stress driven homogenization approach is used, allowing for strict control over both triaxiality and Lode angle. Furthermore, parametric studies are conducted in terms of the void geometry, porosity, triaxiality and Lode angle. The results obtained are then used to critically assess analytical models available in the literature (e.g. [3]).

[1] Luo T., Gao X., 2018. On the prediction of ductile fracture by void coalescence and strain localization. Journal of the Mechanics and Physics of Solids 113, 82-104.

[2] Zhou J., Gao X., Hayden M., Joyce J. A., 2012. Modeling the ductile fracture behavior of an aluminum alloy 5083-H116 including the residual stress effect. Engineering Fracture Mechanics 85, 103-116.

[3] Mbiakop A., Constantinescu A., Danas K., 2015. An analytical model for porous single crystals with ellipsoidal voids. Journal of the Mechanics and Physics of Solids 84, 436-467.

Computational Aspects on the Constitutive Modelling of Multiphase Alloys

M. Vieira de Carvalho[1], D. de Bortoli[2] and F.A Andrade Pires[3]

[1]FEUP, University of Porto, mvcarvalho@fe.up.pt

[2]INEGI, University of Porto, ddbortoli@fe.up.pt

[3]FEUP, University of Porto, fpires@fe.up.pt

Multiphase alloys, such as TRIP (transformation induced plasticity) and dual-phase steels, enjoy considerable technological importance, due to their increased strain hardening capacity, i.e. the combination of high yield strength and elongation at failure. However, the complex microstructural phenomena involved – such as plastic slip and martensitic phase transformations – pose a number of computational challenges.

In this work, several aspects of the computational treatment of constitutive models for such materials are explored, using a crystal plasticity-like model accounting for both plastic slip and martensitic transformations [1]. The model's evolution equations are solved using a fully implicit algorithm that employs a volume-preserving exponential map integrator [2], which is critical for the accurate modelling of incompressible plastic deformations. A rate-dependent regularisation [3] to the original equations is pursued to circumvent a number of difficulties appearing in the elastoplastic formulation, including: non-smooth yield functions, non-unique solutions and, in particular, the formulation of robust algorithm for determining the incremental set of active slip and transformation systems.

The ensuing numerical difficulties – primarily due to the well-documented equation stiffness in the rate-independent limit of vanishing viscosity parameters – are addressed with a number of algorithmic strategies. These include a consistent sub-stepping scheme at the stress update level, the iterative variation of rate-sensitivity material parameters, a procedure to remove the rate dependence of the regularised viscoplastic formulation, and the integration of the critical resolved stress evolution using a generalised mid-point rule.

The formulation presented is exactly linearised, at both the local (stress update) and global level, so that quadratic rates of assymptotic convergence are possible when using a Newton-Raphson scheme in a finite element solution. The impact of the strategies adopted in the overall efficiency and accuracy of the numerical solution to the constitutive equations is assessed in a number of examples, including the macroscopic response of polycrystalline RVEs.

References:

[1] D. de Bortoli, F. Adziman, E.A. de Souza Neto, F.M. Andrade Pires, "Constitutive modelling of mechanically induced martensitic transformations: Prediction of transformation surfaces", Engineering Computations, 35, 772–799 (2018).

[2] 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).

[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).

A Finite-Strain Elasto-Viscoplastic Model for Rubber Toughened Glassy Polymers: Formulation and Validation

Bernardo P. Ferreira[1], S. M. Mirkhalaf [2], Francisco M. Andrade Pires[1]

[1]Department of Mechanical Engineering, Faculty of Engineering, University of Porto,

bpferreira@fe.up.pt, fpires@fe.up.pt

[2]Chalmers University of Technology, University of Gothenburg,

m.mirkhalaf@gmail.com

Over recent years, the modeling of heterogenous multi-phase materials has been a topic of extensive research by the scientific community. Among other approaches, computational homogenization-based multiscale 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.

A considerable effort has been made by the scientific community to develop constitutive models that are able to accurately describe the deformation behaviour of polymeric based materials. Concerning their fracture thoughness, it is well known that glassy polymers show brittle behaviour, particulary under specific conditions such as low temperatures and high strain rates. One important and well-known technique to improve their fracture toughness is termed rubber toughnening, which consists in dispersing rubbery particles in the polymeric matrix in order to hinder the propagation of microfractures. Associated with these rubbery particles is the phenomenon of internal cavitation, meaning that they will behave as voids during the deformation of the rubber toughened polymer.

Polimeric based materials have been studied and modeled at different scales in order to capture their complex deformation behaviour. This model fully couples the finite strain elasto-viscoplastic constitutive model proposed by Mirkhalaf et al. [1] with the yield surface of the well-known micromechanical void growth model proposed by Gurson [2]. In the first place, several parametric studies are conducted in order to verify if the model is able to capture the main features of the rubber toughened glassy polymers characteristic behaviour. The predictive ability of the continuum model is then assessed by comparison with the homogenized response of a voided representative volume element, obtained with a first order homogenization-based multiscale model [3].

[1] Mirkhalaf, S. M., Pires, F. M. A., and Simoes, R. (2016). An elasto-viscoplastic constitutive model for polymers at finite strains: Formulation and computational aspects. Computers and Structures, 166:60–74.

[2] 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.

[3] Reis, F.J.P. & Andrade Pires, F.M. (2013). An Adaptative Sub-incremental Strategy for the Solution of Homogenization-based Multi-scale Problems, Computer Methods in Applied Mechanics and Engineering, Vol. 257, pp. 164– 182.

PGD based domain decomposition method applied to parameterized seismic models

Prattya Datta[1,2], David Modesto[1,2], Josep De La Puente[2] and José María Cela Espín[1,2]

[1]Universitat Politècnica de Catalunya

[2]Barcelona Supercomputing Center

prattya.datta@bsc.es

One of the key steps to generate a seismic image is to solve the parametric Helmholtz equation iteratively. A typical Helmholtz model is solved in a spatial dimension of 10-15 kms and high frequencies. Solving such a large scale model for different parameters requires extensive computations and hence an extremely resource intensive process. The proper generalized decomposition (PGD) technique can be used to accelerate this iterative process by means of real-time evaluations of a surrogate Helmholtz model. Unfortunately, standard PGD methods applied to wave problems are extremely penalized if the global parametric domain imposes large variations along the frequency dimension. More precisely, PGD convergence to a global solution usually fails even when optimized algorithms for non-hermitian problems are applied. This can preclude their application when realistic geophysical models are of concern.

In order to circumvent this issue, a first approach to combine domain decomposition (DDM) and PGD methods is presented for 2D spatial Helmholtz models. This strategy computes local surrogate models that retain the PGD convergence in spatially-decomposed domains, whereas the global convergence of the solution remains guaranteed by the choice of a proper spatial DDM strategy. In particular, the DDM transmission conditions on the boundaries of the sub-domains in the PGD model are defined by overlapped perfectly matched layers (PML). Overlapping PML transmission conditions in full order simulations have shown better global iterative convergences in the residual update, and also better endurance against dependencies on the number of selected sub-domains. Each sub-domain is solved in the reduced order space using the transmission conditions of PML. The global surrogate model is finally built by adding the spatial contribution of all the sub-domains. This process can be ensembled either in serial or parallel approach if HPC resources are available.

Fully coupled multi-scale finite element analysis of TRIP-assisted multi-phase alloys

D. de Bortoli[1,2], M. Vieira de Carvalho[1], I.A. Rodrigues Lopes[1], F.M. Andrade Pires[1]

[1] Computational Multi-Scale Modelling of Solids and Structures Research Group (CM2S), University of Porto, Porto, Portugal

[2] Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI), University of Porto, Porto, Portugal

{ddbortoli, mvcarvalho, ilopes, fpires}@fe.up.pt

With the ever-increasing demand for materials with improved performance, alloys such as advanced high-strength steels (AHSS) enjoy particular technological importance. This is due to their unusually favourable mechanical properties, such as a combination of both high strength and good ductility. To achieve that, these alloys exploit complex micro-structural phenomena, such as the *transformation-induced plasticity* (TRIP) effect, where mechanically induced phase transformations lead to increased overall strain hardening capability. From a modelling perspective, this interplay of deformation mechanisms across multiple phases and length scales is challenging. Capturing the complex material behaviour requires microstructure-aware models capable of reproducing fine-scale crystalline features. In this context, multi-scale models fit naturally, given their ability to both capture fine-scale crystalline features and relate them to the macroscopic, engineering scale.

Based on a recently proposed constitutive model for mechanically-induced phase transformations [1], a unified crystal-plasticity framework is used in this work to model the simultaneous evolution of crystallographic slip and martensite formation in metallic alloys. The constitutive model for mechanically induced phase transformations is based on a classical energy-based criterion for the martensite onset [2], generalised to multi-axial stress states and finite strains. The well-established Phenomenological Theory of Martensite Crystallography [3] is used to derive lattice-scale data on crystallographic transformation systems, which is used by the continuum, grain-scale model. Austenitic slip is modelled using a classical multi-surface crystal plasticity model, and the effects of anisotropic cubic elasticity are also taken into account.

Fully coupled, full-field two-scale finite element analyses (FE^2) are used to reproduce a series of structural experimental results for materials such as austenitic stainless steels and multi-phase TRIP steels, under a wide variety of loading conditions. The constitutive model is calibrated from micro-scale experiments performed on individual phases of TRIP steels. RVE size effects in such alloys are also investigated using a second-order homogenisation scheme. Results show that the proposed framework captures the experimentally observed material behaviour, such as the role of martensitic transformations in the overall mechanical response, highlighting the promise of the multi-scale approach in the modelling and design of advanced materials.

References

[1] D. de Bortoli, F. Adziman, E.A. de Souza Neto, F.M. Andrade Pires, "Constitutive modelling of mechanically induced martensitic transformations: Prediction of transformation surfaces", Engineering Computations, 35, 772–799 (2018).

[2] J.R. Patel, M. Cohen, “Criterion for the action of applied stress in the martensitic transformation”, Acta Metallurgica, 1 (5), 531–538 (1953).

[3] M.S. Wechsler, D.S. Lieberman, T.A. Read, “On the theory of the formation of martensite”, Transactions of AIME, 197, 1503–1515 (1953).

Computational methods for hybrid multiscale modelling in immunology

Dmitry Grebennikov [1,2], Gennady Bocharov [2]

[1]Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia

[2]Institute of Numerical Mathematics of the Russian Academy of Sciences, Moscow, Russia

dmitry.ew@gmail.com, bocharov@m.inm.ras.ru

The immune system is regulated by multiple processes at the genetic, cellular, tissue, organ and the whole organism scales. Therefore, its resulting complexity should be analyzed with hybrid multi-scale models. Virus-host interactions are widely modelled with ODE systems, and interacting components are treated as continuous variables. This approximation is correct only when the numbers of all variables are large enough, whereas the numbers of virions and infected cells are typically small at the initial stage of infection. To efficiently account for their discrete stochastic nature at the early stage, we developed an algorithm for hybrid modelling which utilizes the deterministic representation at the later stages [1].

We present a multiscale hybrid modelling approach which extends the initial model developed for analysis of HIV infection [2]. The multiscale model incorporates the spatio-temporal dynamics of immune cells, viruses and cytokines in lymphoid tissue and couples it with the virus- and cell population dynamics in blood. The locomotion of immune cells is governed by the force-based particle model which accounts for intercellular interactions, cellular intrinsic motility and viscous dissipation. The extracellular dynamics of cytokines is modelled with reaction-diffusion equations. Intracellular HIV replication and molecular regulation is described with ODE systems, and is coupled to the extracellular cytokine fields. Cell fate determining decisions depend on the concentrations of intracellular factors. The model is used to predict the requirements for the containment of HIV infection in local environments of lymphoid tissue. The research is funded by the Russian Science Foundation (grant 18-11-00171).

1. Sazonov I, Grebennikov D, Kelbert M, Bocharov G. *MMNP* (2017) **12**:63–77.

2. Bocharov G, Volpert V, Ludewig B, Meyerhans A. *Springer*, 2018, 221–242.

Multiscale stochastic simulations using a MFH model constructed from full-field SVE realizations

Juan Manuel Calleja Vázquez [1 2], Ling Wu [1], Van-Dung Nguyen [1], Ludovic Noels [1]

[1]Université de Liège

[2]jmcalleja@uliege.be

Nowadays experimental testing of composite materials represents a big challenge for companies, as a large number of tests are necessary to fully characterize a material. Virtual testing represents one of the best options for reducing dramatically these costs in the near future.

In order to make virtual testing become a real alternative for industry when characterizing the performance of a material, it is important not only to have a good representation of its deterministic behaviour, but to take into account all the stochastic non-determinisms that can be present in it: for example geometry variations in the microstructure due to the diposition of the fibers.

In this paper, an inverse Mean-Field Homogenization (MFH) model of a UD composite material used in industry is built from the homogenized stochastic behavior obtained by performing full-field simulations of Stochastic Volume Element (SVE).

As a first step, a micro-mechanical model of reinforced polymer failure with length scale effects is used to simulate the results obtained in tensile tests at constant speed rate of the epoxy used for the construction of the UD material. To this purpose, the complex polymer behavior is represented by a hyperelastic viscoelastic-viscoplastic constitutive model enhanced by a multi-mechanism nonlocal damage model (1). This law is composed of three components: hardening, saturation and failure laws. The characterization of the numerical parameters of the epoxy are obtained by simulating the experimental tensile test and matching the experimental energy release rate (G_c) of the material as developed in (2).

Once the micro-mechanical model of the epoxy is characterized, multiple full-field simulations of composite Stochastic Volume Element (SVE) realizations are performed to characterize the homogenized stochastic behavior of the composite,

information that will be used to build a MFH model as developed in (3). Once this model is constructed, efficient macro scale simulations of a ply failure taking into account geometrical variabilities of the microstructure are possible, bringing the industry closer to a possible future virtual testing of composite materials.

Bibliography

1. *A large strain hyperelastic viscoelastic-viscoplastic-damage constitutive model based on a multi-mechanism non-local damage continuum for amorphous glassy polymers.* **Nguyen, Van-Dung, et al.** 2016, International Journal of Solids and Structures, pp. 192 - 216.

2. *A micro-mechanical model of reinforced polymer failure with length scale effects and predictive capabilities. Validation on carbon fiber reinforced high-crosslinked RTM6 epoxy resin.* **Nguyen, Van-Dung, Wu, Ling and Noels, Ludovic.** 2019, Mechanics of Materials, pp. 193 - 213.

3. *An inverse micro-mechanical analysis toward the stochastic homogenization of nonlinear random composites.* **Wu, Ling, et al.** 2019, Computer Methods in Applied Mechanics and Engineering, pp. 97 - 138.

Simulation of adhesive squeeze flow using smoothed particle hydrodynamics

Lorraine A. Silva[1], Christine Espinosa[1], Lucas F.M. da Silva[2], Eric Paroissien[1], Frédéric Lachaud[1]

[1] Institut Clément Ader (ICA), Université de Toulouse, ISAE-SUPAERO, INSA, IMT MINES ALBI, UTIII, CNRS, 3 Rue Caroline Aigle, 31400 Toulouse, FranceInstitut Clément Ader (ICA)

[2] Department of Mechanical Engineering, University of Porto, 4200-465, Portugal

lorraine.silva@isae-supaero.fr; christine.espinosa@isae-supaero.fr; lucas@fe.up.pt; eric.paroissien@isae-supaero.fr; frederic.lachaud@isae-supaero.fr

In the last few years, so important than an optimized assembly is the Design for Disassembly or Demise (D4D). This conception has been implemented in many industries, for example, in the automobile with the recycling, recovery and reuse of End-of-Life Vehicles (ELVs) [1] and in the aerospace with the processing of the remaining materials for future aircrafts or other industrial applications [2]. Besides, even with the significant progress in that field there are some still recycling challenges, as examples, composite materials and polymers.

Among the many procedures for disassembling materials presented in the literature, the technique using Thermally Expandable Particles (TEP) developed by the FEUP is attractive due to its large potential application field [3]. The process of assembly can be divided into four steps: preparation, application, approach and curing. During the approach, the initial spot of adhesive is squeezed between the substrates. Depending on its compressibility, viscosity and on the roughness of the substrates, the final form of the adhesive will take and keep the shape of the mold, or even bleed in the free space between the substrates [4]. In the first case the thickness and even the particle distribution will be approximately uniform in the squeezed zone while they will not, may be, in the second case.

In this work we are interested in the simulation of the approach to predicting the final form of the adhesive using the smoothed particle hydrodynamics (SPH). The SPH is a meshfree method proposed by Gingold and Monaghan in 1964 [5] which has been the purpose of a lot of enhancements and represents today an elegant alternative solution for numerical simulations of fluids [6]. Simulating free surface movements or possible separation or mixture of different fluids is indeed very easy because the SPH

method is a mesh free technique that computes interactions between particles in a local neighborhood at chosen interval during deformation of the material.

The knowledge of the approach process allows addressing the squeeze flow problem in order to optimize the adhesive final distribution and the TEPs distribution and in the future the disassembly optimization.

[1] LU, Y., BROUGHTON, J., & WINFIELD, P. (2014). A review of innovations in disbonding techniques for repair and recycling of automotive vehicles. International Journal of Adhesion and Adhesives, 50, 119-127. https://doi.org/10.1016/j.ijadhadh.2014.01.021

[2] SABAGHI, M., CAI, Y., MASCLE, C., & BAPTISTE, P. (2016). Towards a sustainable disassembly/dismantling in aerospace industry. Procedia CIRP, 40, 156-161. https://doi.org/10.1016/j.procir.2016.01.088

[3] BANEA, M. D., DA SILVA, L. F., CARBAS, R. J. C., & DE BARROS, S. (2017). Debonding on command of multi-material adhesive joints. The Journal of Adhesion, 93(10), 756-770. https://doi.org/10.1080/00218464.2016.1199963

[4] ENGMANN Jan, SERVAIS Colin, BURBIDGE Adam S. (2005). Squeeze flow theory and applications to rheometry: A review. Journal of Non-Newtonian Fluid Mechanics, 132(1-3), 1-27. https://doi.org/10.1016/j.jnnfm.2005.08.007

[5] GINGOLD, R. A., & MONAGHAN, J. J. (1977). Smoothed particle hydrodynamics: theory and application to non-spherical stars. Monthly notices of the royal astronomical society, 181(3), 375-389. https://doi.org/10.1093/mnras/181.3.375

[6] LIU, G. R. & LIU, M. B. (Ed.). (2003). Smoothed particle hydrodynamics: a meshfree particle method. World Scientific. https://doi.org/10.1142/5340

A Thermo-Mechanically Coupled Cutting Simulation of Ti-6Al-4V Using Advanced Meshless Methods

M. Afrasiabi[1,2], M. Roethlin[1], H. Klippel[1,] K. Wegener[1]

[1] *ETH Zurich, Institute of Machine Tools & Manufacturing (IWF)*
[2] *ETH Zurich, Chair of Structural Mechanics & Monitoring at IBK*

Correspondence to: afrasiabi@ethz.ch

Metal cutting is an operation by which a layer of unwanted material from a given workpiece is removed. It remains one of the most important processes in today's manufacturing science and technology. Merchant [1] claimed in 1998 that up to 15% of the added production value of developed countries is associated with metal cutting operations. Hence, understanding such a process and optimization thereof plays an indispensable role in the advancement of new technologies and developments.

Despite their valuable insights into a better understanding of the mechanism, experimental studies do not suffice as adept tools for analyzing due to many reasons. The process is strictly dominated by large deformations and gradients, new surface generation, and extremely high strain rates, to name a few. On the other hand, the analytical solution to most of these operations does not exist, or in the best case scenario, is far from trivial. This investigation leaves the researchers with the simulation of the process.

Finite Element Method (FEM) has already established itself as the most popular choice for the simulation of metal cutting. However, it is nearly impossible nowadays to find a robust FEM solver that does not rely on adaptive remeshing procedures. Excellent accounts in this regard can be found in [2] and [3]. To release this cumbersome, and computationally expensive, procedure, a completely different approach can be considered which enables the spatial discretization using some Lagrangian points, called particles. The essential characteristics of the meshfree particle methods are that there is no need for a highly structured mesh as required in FEM. The most widely-used meshfree method to date is perhaps the Smoothed Particle Hydrodynamics (SPH) which was simultaneously introduced by Lucy [4] and Gingold et al. [5] in the late 70s.

In this work, a particle-based framework is developed to model a 2D orthogonal cutting of Ti-6Al-4V. To this end, a set of stabilization terms in addition to some corrective schemes are employed in an updated Lagrangian frame. Together with the stabilized SPH algorithm for the mechanical solver, a Particle Strength Exchange (PSE) method [6,7] is used for the heat conduction and thermal modeling. This choice is made based upon a great accuracy-performance trade-off that PSE offers in the discretization of higher-order derivatives, e.g., the Laplacian operator in the heat equation.

Yet another contribution of the present work lies in the adoption of a modified Johnson-Cook flow stress model, suggested by Sima et al. [8]. Motivated by the experimental and numerical results presented by the authors of [8], this constitutive model is herein chosen to capture the strain softening effect in the machining of titanium alloys. As illustrated in Figure 1, the proposed meshless solver is perfectly capable of representing the adiabatic shear bands and chip formation even in relatively low-resolutions. The results obtained from the meshless simulation stays in a good agreement with the available FEM and experimental data.

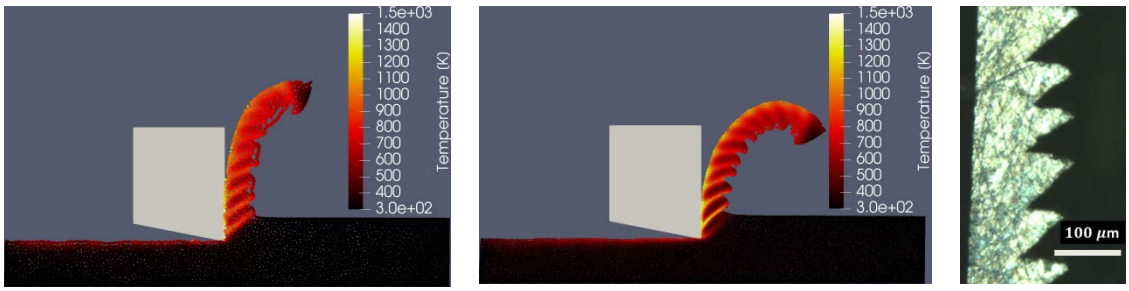


Figure 1. Temperature distribution and chip formation using the present method in low (left) and medium resolutions (middle). The chip shape (right) in experiment by [8].

Selected references

[1] M. Merchant, “An interpretive look at 20th century research on modeling of machining,” Machining Sc & Tech., 1998.
[2] P. Arrazola et al., “Recent advances in modelling of metal machining processes,” CIRP Annals-Manf., 2013.
[3] T. Marusich et al., “Modelling and simulation of high-speed machining,” IJNME, 1995.
[4] L. B. Lucy, “A numerical approach to the testing of the fission hypothesis,” The astronomical journal, 1977.
[5] R. A. Gingold and J. J. Monaghan, “Smoothed particle hydrodynamics: theory and application to nonspherical stars,” Monthly notices of the royal astronomical society, vol. 181, no. 3, pp. 375–389, 1977.
[6] S. Mas-Gallic and P. Raviart, “Particle approximation of convection-diffusion problems,” *Report of Univ de Paris*, 1986.
[7] J. D. Eldredge, et al., “A general deterministic treatment of derivatives in particle methods,” *JCP*, 2002.
[8] M. Sima and T. Özel, “Modified material constitutive models for serrated chip formation simulations and experimental validation in machining of titanium alloy ti–6al–4v,” *International Journal of Machine Tools and Manufacture*, 2010.

Multiphysics Simulation of Laser Metal Deposition Manufacturing Process Using a Meshless Method

Boussad Abbès [1], Fazilay Abbès [1], Tahar Anedaf [1], Yuming Li [1]

[1]GRESPI, University of Reims Champagne-Ardenne

boussad.abbes@univ-reims.fr, fazilay.abbes@univ-reims.fr, tahar.anedaf@etudiant.univ-reims.fr, yuming.li@univ-reims.fr

Laser Metal Deposition (LMD) is one the additive laser manufacturing technologies for obtaining complex metallic shapes and tools by adding lased material powder on a substrate. Furthermore, it has found an important application niche in the coating or repair of high value components as well as components that have undergone significant wear. It is used for example to repair turbine blades for the aerospace industry, drill pipes for offshore industry, injection molding tools for the automotive industry among others. To control the manufacturing process and the influence of the operating parameters on the final characteristics of the fabricated parts, it is important to understand the complex mechanisms involved in their manufacturing. Therefore, computational simulation has an important role to play in addressing these challenges.

This paper presents a three dimensional multi-physics models to describe the physical mechanism of heat transfer, melting and solidification that take place during the LMD process. The simulated transient temperature profile, the geometrical features of the generated structures and thermal cycles are presented. The results obtained from the model based on the meshless Finite Pointset Method (FPM), which is a variant of the Smooth Particle Hydrodynamics (SPH) method, provide the basis for the selection of the process parameters in additive manufacturing.

Micromechanical Modeling and Estimation of Elastic Properties of Pure MXene ($Ti_3C_2T_x$) Films

Krzysztof Grabowski [1] Shreyas Srivatsa [2] Tadeusz Uhl [3]

[1,2,3] AGH University of Science and Technology, Krakow, Poland

kgrabow@agh.edu.pl

MXenes are 2-dimensional (2D) materials made of metal carbides or metal nitrides. They have found a wide range of applications because of its hydrophilic and metallic behavior due to its surface termination and transition metal atoms, respectively. MXenes, particularly Titanium Carbide (Ti_3C_2) with surface termination (T_x) ($Ti_3C_2T_x$), have been used to fabricate pure MXene films and MXene/PVA nanocomposite. The MXene ($Ti_3C_2T_x$) monolayer (flake) elastic properties and Young's modulus (in the range of 300-360 GPa) are reported in the literature from Molecular Dynamics results and nanoindentation tests. The MXenes flakes stack up, one on top of the other, to form pure MXene film. Though limited experimental results are available in the literature, both analytical and numerical models for the pure MXene film are to be developed for the purpose of mechanical property estimation.

The focus of the paper is on the micromechanical modeling of pure MXenes ($Ti_3C_2T_x$) and estimation of the elastic properties of the MXene stack. MXenes are modeled as thin plate structures in microscale as the lateral dimensions of the MXene flakes are in the range of 2-10 microns and the thickness is in the range of 1-2 nanometers.

First, an analytical method is used to perform investigations. Classical Laminate Plate Theory (CLPT) which is based on Kirchhoff's plate theory assumptions, is used to model the MXene stack which forms the pure MXene film. The stiffness matrix and Young's modulus of the MXene stack are estimated based on this analytical model. The bonding between one MXene flake to another plays a crucial role in the estimation of Young's modulus of pure MXene stack. Therefore, in this paper, the bonding layer between the MXene flakes is considered and is termed as an interface layer. The Young's modulus of this interface layer is estimated based on the overall MXene stack Young's modulus reported in the literature on MXene films. The effect of the geometric and

material properties of the interface layer on the overall pure MXene stack elastic properties is studied.

Second, pure MXene is subjected to numerical modeling and analysis using Finite Element Method. They are modeled as a single layer, double layer and stack of MXenes with interface between them. The models are subjected to tensile loads in-plane with the MXene. The results of the simulations are reported in this paper. The results indicate a future work that the interface layer properties and behavior between MXene flakes need detailed modeling in the sub-micron scale using Molecular Dynamics which can improve the micromechanical model estimation.

Computational study of deformation mechanisms in hcp metal: Application to pure zinc

Fazilay Abbès [1], Nhan P. T. Nguyen [1, 2], Jean-Sébastien Lecomte [3], Christophe Schuman [3], Boussad Abbès [1]

[1]GRESPI, University of Reims Champagne-Ardenne,
[2]University of Danang, [3]LEM3, University of Lorraine

fazilay.abbes@univ-reims.fr, pham-the-nhan.nguyen@etudiant.univ-reims.fr, jean-sebastien.lecomte@univ-lorraine.fr, christophe.schuman@univ-lorraine.fr, boussad.abbes@univ-reims.fr

Zinc metal is well-known for its high corrosion resistance in most environments, which accounts for its successful use as a protective coating on a variety of products and in many exposure conditions, especially in automotive and building applications. Zinc has a hexagonal close-packed (hcp) crystalline structure. Compared to other hcp metals like titanium or magnesium, zinc exhibits a strong anisotropic behavior. Due to the lack of adequate constitutive laws, hcp sheet forming finite-element simulations have been generally performed using classical macroscopic anisotropic criteria for cubic metals. Recent advances in the formulation, numerical implementation, and validation of macroscopic plasticity models for hcp materials have allowed a better capture of specific features like the anisotropy and the tension-compression asymmetry in yielding of hcp metals.

A more relevant approach is the physically-based one, which requires a good understanding of the deformation mechanisms at the individual grain-scale in the polycrystalline sample. Moreover, depending on its orientation, the grain response involves different slip systems activity rates. Indeed, an accurate determination of slip resistance and its evolution, that is hardening, is of prime importance to well predicting the macroscopic response of a polycrystalline specimen.

This work details such approach in the case of a pure polycrystalline zinc sheet. Experimental data, issued from instrumented indentation tests performed on grains of distinct crystallographic orientations is used. Combining crystal plasticity finite element method (CPFEM) with an inverse identification, we have determined the unknown

critical resolved shear stresses. We have also investigated the orientation-dependent characteristics under complex and local loading conditions such as those involved in a nanoindentation test. Indeed, the complexity of the stress state that develops underneath the indenter depends on the geometrical characteristics of the latter and the crystallographic orientations of the grains, which can give rise to different interactions between the deformation modes.

Multiphysical simulation of aluminum panels' behaviour hit by lightning strikes

Christine Espinosa [1], Florent Grotto [1], Stéphane Vilcocq [2], Frédéric Lago [2], Thomas Montel[1], Oscar Gnangnon [1]

[1] Institut Clément Ader, Université de Toulouse, ISAE-SUAPERO, IMT MINES ALBI, UTIII, INSA, CNRS, 3 Rue Caroline Aigle, F-31400 Toulouse CEDEX 04, France

[2] DGA-Techniques aéronautiques, 47, Rue Saint-Jean, 31130 Balma, France

christine.espinosa@isae-supaero.fr

One of the main safety issues facing aircrafts is the protection against lightning strikes. Metallic aircrafts are protected against current flows because of their high electrical conductivity. However, at the arc attachment location, a serious damage may happen and even it may be developed into a perforation. Such perforation in the fuel tanks or close to the energetic materials may jeopardize the safety of the aircraft and the holding of the carriers. Laboratory tests simulating lightning strikes follow standard regulations requirements that prescribe the current waveforms the structure must resist depending on the zone of the airplane. D+B+C* current waveforms are under concern here and are reproduced in by specific current delivery devices at DGA-Ta lightning lab. Sensibility analysis done after experimental variability campaigns on aluminum panels allowed us introducing a Damage Severity Index as a quantitative representation of the severity level of the local damage [1]. Typical local damage are a dome on front face, a double dome on front and rear face, a sharp crater on front and rear face, and a hole, of typical diameters of about 10mm. The DSI showed as expected the major effect of the delivered electrical charge (in Coulombs). The second most active parameter was the position of the hit. In contrary to composite panels [2], it is surprising for metallic plate damage.

It is then of particular importance to understand the contribution of each component of the load on the global behavior of the panel during the lightning in order to understand why local damage is affected.

This talk will present the fully LS-DYNA® electromagnetic-thermal-transient mechanical coupled numerical model that has been developed to represent the D-B-C* loading. Results of numerical simulations are presented for different sets of loadings.

The contribution of each component of the load on the macroscopic panel behavior and maximum local temperature is investigated.

[1] C. Espinosa, I. Alhossen, A. Hor, E. Pierré, S. Vilcocq, R. Chieragatti, T. Montel, O. Gnangnon (2018). Experimental investigation of the repeatability of direct damage induced by lightning strikes on metallic panels. 15th High-Technology Plasma Processes (HTPP15), Toulouse, France.

[2] Y. Duval, A. Bigand (2017). Effect of boundary conditions on damage resulting from a D-waveform on a composite plate. International Conference on Lightning and Static Electrocity (ICOLSE), Nagoya, Japan.

Modelling of honeycomb composite sandwich panel with flax fiber skin

Matteo Riganti[1,2],Frèdèric Lachaud[1],Christine Espinosa[1], Mathieu Boutin[1]

[1] *Institut Clément Ader (ICA), Université de Toulouse, ISAE-SUPAERO, INSA, IMT MINES ALBI, UTIII, CNRS, 3 Rue Caroline Aigle, 31400 Toulouse, France*

[2] *POLITECNICO DI MILANO, Piazza Leonardo da Vinci, 32, 20133 Milano, Italia*

frederic.lachaud@isae-supaero.fr

riganti.matteo@outlook.it

A study over a flax fiber sandwich and a honeycomb/E-glass fiber sandwich (standard aeronautic sandwich cabin panel) is conducted in order to trace and compare their response behavior, under static and dynamic loads (impact). Firstly, skin and core are taken into consideration separately. For the skin, realized by fabric plies, a damage model [4] developed in precedent study [2] is applied. For Nomex® honeycomb, experimental tests are realized (fig.1) to understand overall behavior [1,3], and after the influence of geometrical local imperfections due to manufacture process, and of uncertainties in mechanical properties, is taken into account. Different FEM models (fig.2) are realized and set in order to fit experimental curves (fig.3). Through a variability analysis, mesh influence is investigate randomly displacing nodes and its consequence over instability phenomena will be evaluated, while the effect of mechanical property uncertainties is investigated using a parametrical approach.

Figure 1: Experimental crushing of Nomex® honeycomb

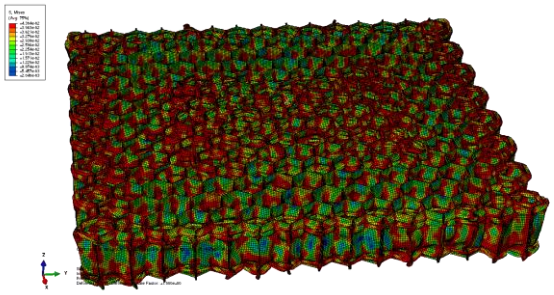


Figure 2: FEM simulation of honeycomb compression

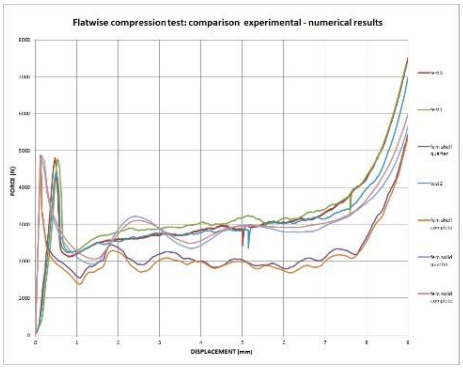


Figure 3:Experimental curve flatwise compression test

Acknowledgement: thanks to VESO-CONCEPT for materials supply.

References:

[1] M. Giglio, A. Manez, A. Giglioli, *Investigations on sandwich core properties through an experimental–numerical approach*, Politecnico di Milano, Composites: Part B 43 (2012) 361–374

[2] F. Lachaud, C. Espinosa , L. Michel ,P. Rhame, R. Piquet, *Modelling Strategies for Simulating Delamination and Matrix Cracking in Composite Laminates.* Applied Composites Materials. DOI 10.1007/s10443-014-9413-4, August 2014

[3] D. Mohr, M. Doyoyo, *Deformation-induced folding systems in thin-walled monolithic hexagonal metallic honeycomb*, MIT, U.S.A., International Journal of Solids and Structures 41 (2004) 3353–3377

[4] C.G. Skamniotis, M. Elliott, M.N. Charalambides, *On modelling the constitutive and damage behaviour of highly non-linear bio-composites – Mesh sensitivity of the viscoplastic-damage law computations*, Imperial College London, International Journal of Plasticity 114 (2019) 40–62

Probablistic approach of a dynamic analysis of wind turbine on flexible foundation

Abderraouf Kamel[1,2] . Abdelkhalak El Hami[1] . Mounir Ben Jdidia[2] . Lotfi Hammami[2] . Majdi Yangui[2]. Mohamed Haddar[2] .

[1]Laboratory of Mechanics of Normandy (LMN), National Institute of Applied Sciences of Rouen, Rouen, France.

[2]Laboratory of Mechanics, Modeling and Manufacturing (LA2MP), Mechanical Engineering Department, National School of Engineers of Sfax, Sfax, Tunisia

abderraouf.kamel @insa-rouen.fr

In this paper, a dynamic analysis of a wind turbine in flexible base is carried out and combined with a stochastic analysis to investigate the robustness of the system. Climatic properties and geotechnical properties are chosen as random variable.in fact,for this analysis, a finite element model with Matlab software of horizontal axis wind turbine rated at 500 kW is elaborated. Fig1

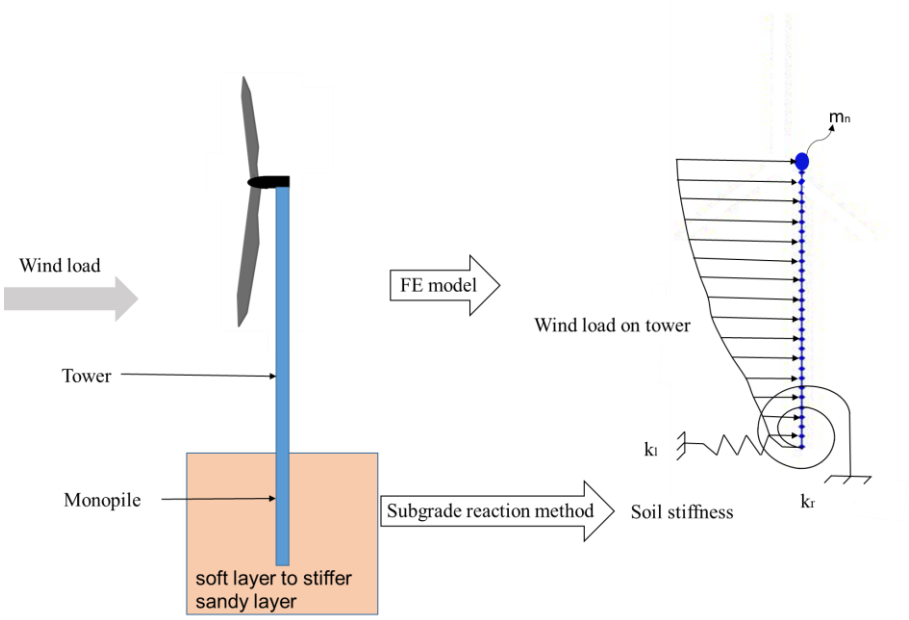


Figure 1 A the FE model of a wind turbine with monopole foundation

In this work, the tower was considered as regular column with a top mass. The properties of the turbine tower are summarized in Table 1.

Table 1 design parameters of the turbine tower

Parameters	Description	Values
D_T	tower diameter	2.5 m
e_T	tower thickness	0.012 m
E_T	Young's modulus	$2.1\ 10^{11}$ Pa
ρ_T	Mass density	7800 kg/m^3
V_{10}	the wind speed at the height 10 m	10 m/s
m_n	Mass of the nacelle	32 000 Kg
	Rated power	500 KW

Monopile is used to support this slender structure. The subgrade reaction method is used to model the soil-structure-interaction (SSI) [1].in this method, pile-soil is substituted by a lateral spring and another rotation. Wind action is then applied to the wind turbine.

Wind velocity v_{10}, lateral stiffness k_l and rotational stiffness k_θ of the foundation are chosen as random variables that will be used in the stochastic study of the system.

In this study, the results of MC simulation [2], which will be considered as a reference, are compared with that of gPC simulation [3]. It has been found that gPC simulation almost reproduces the results of MC simulations for a small standard deviation ($\sigma_{v10}= \sigma_{kl} =\sigma k_\theta =5\%$) with a second-order polynomial. For a higher standard deviation ($\sigma_{v10}= \sigma_{kl} =\sigma k_\theta =10\%$) a, six-degree polynomial is sufficient to produce accurate results.

Knowing that the gPC simulations are accompanied by a phenomenal reduction in computing time compared with MC simulations, this technique then presents an effective and powerful tool for studying the robustness of the structure for this type of problems.

References

[1] S. Adhikari et S. Bhattacharya, «Dynamic analysis of wind turbine towers on flexible foundations,» *Shock and Vibration*, vol. 19, pp. 37-56, 2012.

[2] Y. A. ,. e. Shreider, The Monte Carlo method: the method of statistical trials, vol. 87, Elsevier, 2014.

[3] D. Xiu et G. E. Karniadakis, «Modeling uncertainty in flow simulations via generalized polynomial chaos,» *Journal of computational physics*, vol. 187, n° %11, pp. 137-167, 2003.

Multi-scale Reliability Based Design Optimisation for Unidirectional FRP Composite Laminates

Sadik Omairey[1], Peter D. Dunning[1], Srinivas Sriramula[1a]

[1]School of Engineering, University of Aberdeen, AB24 3UE
[a]Lloyd's Register Foundation (LRF) Centre for Safety and Reliability Engineering, University of Aberdeen, AB24 3UE
s.omairey@abdn.ac.uk

The full benefits of FRP are often not realised in practice due to conservative safety factors arising from a lack of understanding of how uncertainties affect performance. Therefore, in this study a multi-scale reliability-based design optimisation (RBDO) framework is developed for a unidirectional fibre reinforced polymer (FRP) composite laminate. In terms of reliability, a probabilistic framework, developed by the authors (Omairey et al, 2019, Omairey et al, 2018), that employs a FEA-based surrogate model is used to estimate stiffness properties, while accounting for geometric and material property uncertainties at micro, and meso scales. Using the developed framework, lamina thickness and orientations are optimised to minimise mass, subject to reliability constraints on several stiffness criteria at the laminate scale.

Many of the uncertainties occur due to the multi-scale build-up nature of composites, mainly in material properties and geometric characteristics. These uncertainties present a challenge in estimating composite material properties and conducting reliability-based optimisation. The currently available property estimation/homogenisation tools that are used to carry out reliability analysis and optimisation are mainly divided into two categories: analytical approaches, based on an assumed model configuration, and finite element homogenisation methods that are more flexible and accurate, but computationally expensive. Hence, this study uses a surrogate model based framework utilising numerically homogenised FEA data, which is capable of representing various multi-scale uncertainties. Employing this framework significantly decreases the analysis duration compared with FEA; therefore, it is feasible to conduct multi-scale reliability analysis and reliability-based optimisation of unidirectional FRP composite laminates.

Keywords: Composites; Uncertainty; Homogenisation; Surrogates; Reliability; Optimization.

References

Omairey, S., Dunning, P. and Sriramula, S. (2019). Multiscale Surrogate-based Framework for Reliability Analysis of Unidirectional FRP Composites. Composites Part B: Engineering, [under review].

Omairey, S., Dunning, P. and Sriramula, S. (2018). Influence of micro-scale uncertainties on the reliability of fibre-matrix composites. Composite Structures, 203, pp.204-216.

Efficient structural reliability analysis based on polynomial chaos expansion and maximum entropy method

Jinsheng Wang [1] ; Muhannad Aldosary[2]; Chenfeng Li[1]

[1] Zienkiewicz Centre for Computational Engineering, Swansea University, Swansea, SA1 8EN
[2] Dams and Water Resources Engineering, University of Anbar, Iraq
844051@swansea.ac.uk

Abstract: In the presence of uncertainties, the proper assessment of the failure probability of a structural system is an important component in the modern reliability-based engineering framework. However, the estimation of failure probability of a structural system can generally be computationally demanding, especially for rare failure events where complex finite element models are involved for response evaluation. Therefore, alternative approaches for efficient computation of structural failure probability while retaining high accuracy is of paramount importance to the structural engineering community. Thus, herein this work an efficient hybrid approach is proposed that combines an efficient surrogate model technique with the maximum entropy method (MEM) for accurate failure probability evaluation of a structural system. In the proposed method, the statistical moments of the performance are furnished by the surrogate model, whereas the probability density function (PDF) is constructed using MEM under moment constraints. With the availability of the analytical expression of PDF, the failure probability of the structural system is directly obtained by numerically integrating the PDF over the failure domain. The applicability of the proposed approach is investigated using numerical examples and its performance is compared with Monte Carlo simulation (MCS) and conventional reliability analysis methods, namely first-order reliability method (FORM), importance sampling method (IS) and subset simulation (SS), whenever possible. It is observed that: the proposed method has the capability to fully and accurately capture the uncertainty inherent in the model response with a relatively small number of functional calls, which is more efficient compared with simulation approaches; the proposed method can readily provide failure probability estimation once the PDF is constructed, which is especially attractive when different thresholds are of concern; other efficient surrogate model methods, such as support vector machine, artificial neural network and Kriging, can easily be incorporated into the presented framework for structural reliability analysis, which is the scope of the future research.

Key Words: Structural reliability analysis; Surrogate model; Maximum entropy method; Statistical moments; Probability density function

Performance of drag models in CFD-DEM

Sizeng You [1], Ashutosh Bhokare[1], *Chenfeng Li[1]

[1]College of Engineering, Swansea University, UK

* Corresponding author: c.f.li@swansea.ac.uk

Flows witnessed in nature and the industry rarely involve a single phase. A thorough understanding of multiphase flows is critical to the design, up-scaling, optimisation, and correction of industrial processes. Multiphase flows in which one phase is a fluid and the other is solid-particulate finds applications in fluidised beds, cyclone separators, pneumatic conveyors and other industrial processes. This class of multiphase flows can be modelled using the Eulerian-Eulerian approach in which both the fluid and particulate phases are treated as inter-penetrating continua. Although this approach is able to model macroscopic phenomena it does not capture the local behaviour of particles. In order to accurately model particle motion an alternative Eulerian-Lagrangian approach can be used in which the fluid is treated as a continuum and the solid-particulate as discrete Lagrangian particles interacting with the continuum phase. The discrete element method (DEM) is a numerical technique which describes the motion of discrete particles by solving Newton's second law of motion. The coupling strategy of modelling fluid flow using computational fluid dynamics (CFD), particulate motion using DEM and the interaction between them is referred to as CFD-DEM.

CFD-DEM is considered to be a meso-micro approach in which the fluid phase is modelled at the mesoscopic level and the solid-particulate phase at the microscopic level. The Navier-Stokes equations are used as the governing equations for the fluid phase and can be solved using the finite volume method (FVM). Newton's second law of motion is used as the governing equation for the particles and solved using numerical techniques under DEM. In a complete two-way coupled CFD-DEM scheme the presence of solid phase is considered as a volume fraction field and the Navier-Stokes equations are modified likewise. Newton's third law of motion is obeyed by considering exchange of momentum between the phases. The drag and pressure gradient force are found to be the dominant forces. Thus, an accurate drag model is critical to the accuracy of a CFD-DEM scheme.

This talk introduces the CFD-DEM scheme and all the numerical ingredients needed to successfully implement it. It then introduces the various drag models available in literature and popularly used in CFD-DEM. To compare the performance of the drag models a problem statement is defined in which fluid is forced to flow through a region of stationary particles and the drag on the particles is computed. The results of a purely CFD simulation in which the particles are fully resolved by the FVM mesh is used as the basis of the comparison. CFD-DEM simulations are run using the drag models in the same setup and an attempt to compare their performance at various inlet velocities is made. It is found that at low Reynolds number flows, the drag models contain a constant predictable error while at higher Reynolds number flows the error builds up with the flow rate and is highly unpredictable. Although the error in drag is slightly sensitive to the volume fraction, it does not seem to affect the accuracy by a huge margin for most drag models.

PyEFEM: Massively parallel python based FEM framework for flow problems

Liang Yang [1,2]
[1]School of Water, Energy and Enviroment (SWEE), Cranfield University, Bedford, UK
[2] Department of Earth Science and Engineering, Imperial College London, South Kensington, UK
liang.yang@cranfield.ac.uk

Numerical simulations of complex multiphysics multiscale problems, such as fluid-structure interaction, turbulent flows, which demand fine spatial and temporal resolutions, require often impractical (or unavailable) computing resources. The performance in supercomputing on modern computer architectures is typically restricted by the cost of memory per core. Loading the memory is slower than the performing the arithmetic operations. The matrix-free methods, where matrix-vector product is formed on-the-fly becomes popular, including on GPUs. The Cartesian data structure is much faster than unstructured, as the structured meshes can be easily accessed by the index. Unstructured solver involves an additional cost arising from indirect addressing and non-contiguous memory access.

For these reasons, the explicit stabilised finite element is designed to be a promising algorithm for solving the nearly-incompressible, turbulent flow problems, with reduced memory costs. Implementing the method, PyEFEM is a Python based framework for solving flow problems using matrix-free stabilised finite element, which exhibits excellent scalability on current supercomputing systems for large-scale unsteady flow simulations, reaching up to 10 billion unknowns on HPCs. It is designed for massively-parallel cross-platform and its applications include turbulent flow (See Fig. 1), biological flow, aeroacoustics (See Fig. 2), environmental flow (See Fig. 3), pore scale modelling (See Fig. 4), flow through porous media (See Fig.5) and haemodynamics.

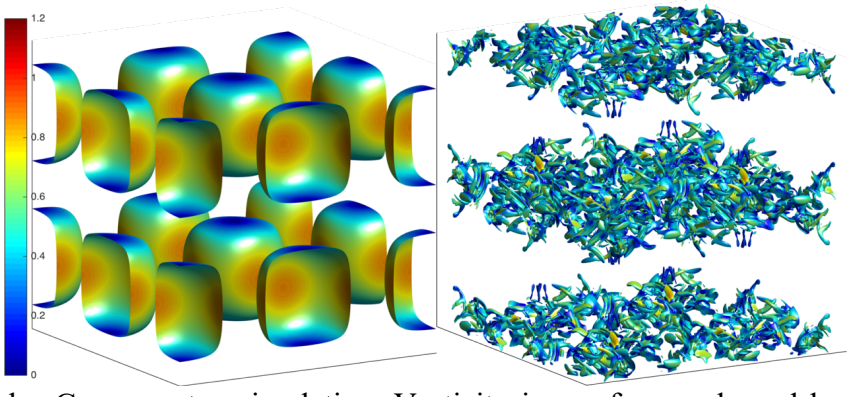


Fig. 1: Taylor-Green vortex simulation. Vorticity iso-surfaces coloured by velocity at different time instances. (left) isosurface for $|\boldsymbol{\omega}|=1$ at t=0; (right) isosurface for $|\boldsymbol{\omega}|=9$ as t=11 [1].

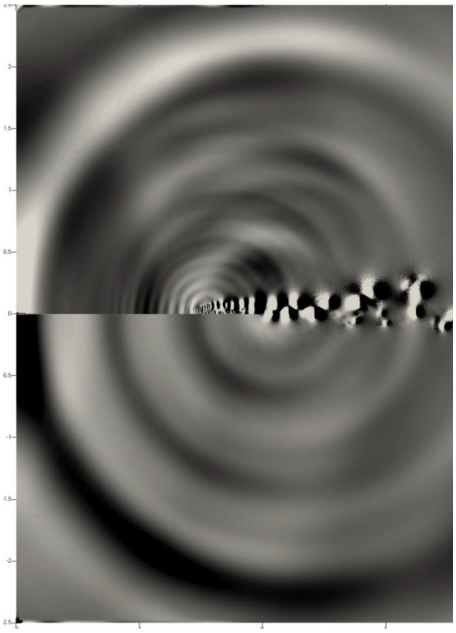


Fig. 2. Dilatation field of a flow over a trailing edge with obstacle with the non-reflecting boundary conditions (NRBCs) [2].

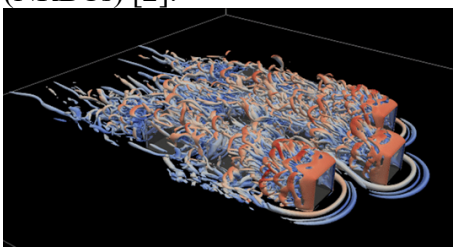


Fig. 3. Urban air flow and natural ventilation problem with PyEFEM.

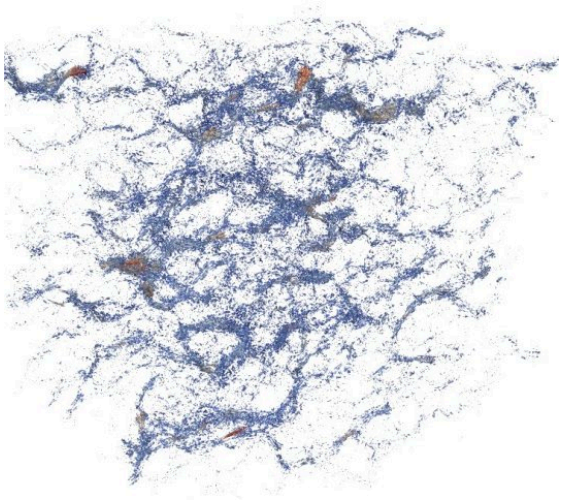


Fig. 4: Pore scale modelling, flow in Berea sandstone.

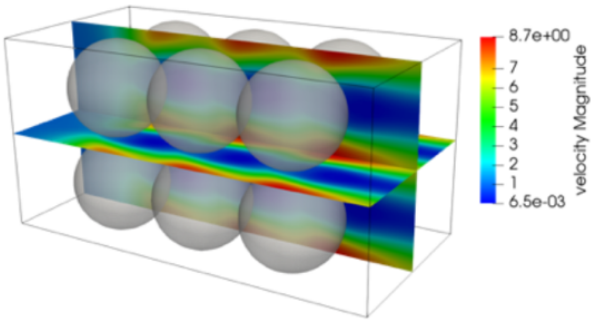


Fig. 5: Flow through a semi-infinite structured array of sphere at Re=18.

This talk will describe recent efforts at developing the matrix-free stabilised finite element models for different applications on cross-platforms. The already effective in-house research code will be taken to the next stage: a strong and versatile tool, with the application to oil & gas, nuclear thermal hydraulics, aerodynamics/noise for trains, automotive and airplanes.

References:

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

[2] Yang, L., et al. Direct numerical simulation of low Mach-number isentropic flow noise using stabilised finite element.

[3] Yang, L., Yang, J., Boek, E., Sakai, M., & Pain, C. (2019). Image-based simulations of absolute permeability with massively parallel pseudo-compressible stabilised finite element solver. Computational Geosciences, 1-13.

The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics

Irina Tezaur [1,*], Alejandro Mota[1], Coleman Alleman[1], Greg Phlipot[2]

[1]Sandia National Laboratories, [2]California Institute of Technology

*ikalash@sandia.gov

Concurrent multiscale methods are essential for the understanding and prediction of behavior of engineering systems when a small-scale event will eventually determine the performance of the entire system. Here, we describe the recently-proposed [1] domain-decomposition-based Schwarz alternating method as a means for concurrent multiscale coupling in finite deformation quasistatic and dynamic solid mechanics. The approach is based on the simple idea that if the solution to a partial differential equation is known in two or more regularly shaped domains comprising a more complex domain, these local solutions can be used to iteratively build a solution for the more complex domain. The proposed approach has a number of advantages over competing multiscale coupling methods, most notably its concurrent nature, its ability to couple non-conformal meshes with different element topologies (Figure 1), and its non-intrusive implementation into existing codes.

In this talk, we will first overview our original formulation of the Schwarz alternating method for multiscale coupling in the context of quasistatic solid mechanics problems [1]. We will discuss the method's proven convergence properties, and demonstrate its accuracy, convergence and scalability of the proposed Schwarz variants on several quasistatic solid mechanics examples simulated using the Albany/LCM code.

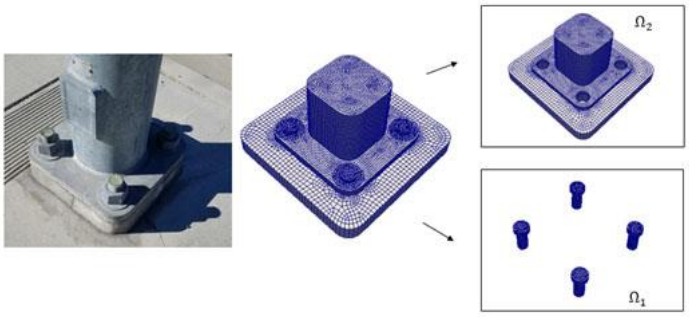


Figure 1: Schwarz Domain Decomposition for Production-Like Bolted-Joint Geometry

The bulk of the talk will present some recent extensions of the Schwarz alternating formulation to *dynamic* solid mechanics problems [2]. Our dynamic Schwarz formulation is *not* based on a space-time discretization like

other dynamic Schwarz-like methods; instead, it uses a governing time-stepping algorithm that controls time-integrators within each subdomain. As a result, the method is straight-forward to implement into existing codes (e.g, Albany/LCM), and allows the analyst to use different time-integrators with different time steps within each domain. We demonstrate on several test cases (including bolted-joint problems of interest to production; e.g. Figure 1) that coupling using the proposed method introduces no dynamic artifacts that are pervasive in other coupling methods (e.g., spurious wave reflections near domain boundaries), regardless of whether the coupling is done with different mesh resolutions, different element types like hexahedral or tetrahedral elements, or even different time integration schemes, like implicit and explicit. Furthermore, on dynamic problems where energy is conserved, we show that the method is able to preserve the property of energy conservation.

REFERENCES

[1] A. Mota, I. Tezaur, C. Alleman. "The alternating Schwarz method for concurrent multiscale coupling", *Comput. Meth. Appl. Mech. Engng.* 319 (2017) 19-51.

[2] A. Mota, I. Tezaur**,** G. Phlipot. "The Schwarz alternating method for dynamic solid mechanics", in preparation for submission to *Comput. Meth. Appl. Mech. Engng.*

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
5	1.1	The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics	**Irina Tezaur** (Sandia National Laboratories)*
8	1.30	Pore Water State in Heated Concrete---Comparing a Numerical Model to NMR Measurements	**Christoph Pohl** (Bundesanstalt für Materialforschung und -prüfung)*
11	2.6	Computationally efficient homogenization for modeling of nonlinear functionally graded materials	**Witold Ogierman** (Silesian University of Technology)*
12	2.28	Multiphysics Computation in Batteries Involving Electromagnetism and Thermomechanics	**Bilen Emek Abali** (TU Berlin)*
18	1.2	On modeling interfaces in composite with multi-physic coupling	**Michele Serpilli** (Università Politecnica delle Marche
20	1.15	Sub-Modeling Approach to Investigate the Cracking Behavior of Reinforced Concrete Structures Considering Polymorphic Uncertainty	**Katharina Kremer** (Ruhr University Bochum)
25	1.7	A computational multi-physics model to predict the chemo-mechanical degradation of historical oil paintings	**Emanuela Bosco** (Eindhoven University of Technology)*
26	1.30	A coupled chemo-mechanical model for biogenic sulfide corrosion in concrete sewer pipes	**Emanuela Bosco** (Eindhoven University of Technology)*

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
27	**1.28**	Degradation of Lithium-Ion Batteries in Aerospace	**Linda J. Bolay** (German Aerospace Center)
28	**1.16**	Reduced-order Modelling Scheme for Problems with Fully Resolved Microstructures Generated by Generalized Periodic Unit Cells	**Martin Doškář** (Czech Technical University in Prague)
31	**1.13**	Fragment size characterization for granular flow in highly damaged ceramics	**Lori Graham-Brady** (Johns Hopkins University)
37	**1.5**	Development of a modified Voronoi's tesselation algorithm for the determination of the effective properties of cork-based composites	**Marco Delucia** (I2M - Institut de mécanique et d'ingénierie - Université de Bordeaux)
39	**3.13**	Data driven computational analysis of open foam materials	**Nanda Gopala Kilingar** (University of Liege)*
41	**1.4**	Simulation Model for Single unit Warpage of Shadow moire in Flip-Chip Process	**Wan-Chun Chuang** (Department of Mechanical and Electromechanical Engineering, National Sun Yat-sen University)
42	**1.19**	Efficient and accurate two-scale FE-FFT-based prediction of polycrystalline material behavior at finite strains	**Christian Gierden** (Institute of Applied Mechanics, RWTH Aachen University)
43	**1.3**	Diffusion-Kinetic Monte Carlo Methods for Neutral	**Bert Mortier** (KU Leuven)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
		Transport in Plasma Edge Simulations of Nuclear Fusion Reactors	
44	**1.6**	Development of a simple ergodic stochastic representative volume element for heterogeneous materials with random geometry of microstructure	**Dmytro Pivovarov** (Chair of Applied Mechanics, Friedrich-Alexander University Erlangen-Nürnberg)
46	**3.3**	Multi-uncertainty analysis of the indentation process of key engineering materials	**Thiago Doca** (University of Brasília)
47	**3.1**	Adjoint Based Optimisation of an Internal Cooling Channel U-Bend	**Jens-Dominik Müller** (Queen Mary, University of London)
205	**Plenary Session**	Multi-scale and Multi-physics challenges for Future Aircraft: A Hierarchical Approach	**Paul G. Tucker** (Cambridge University)
202	**2.29**	Examining the Mutation Effect of SLC26A4 STAS Domain By Observing the Communication Between Secondary Structures	**Hyun Joon Chang** (Korea University);
~~**208**~~	-	~~Probabilistic Design Optimization for CO2 Storage with Leakage Risk Control~~	~~**Ben Mansour Dia** (CPG)*~~
210	**3.11**	Development of Multiscale Multi-physics Based Modelling and Simulations with the Application to	Yizhi Shao (Brunel University)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
		Precision Machining of Aerofoil Structures	
211	3.16	An Investigation of stepwise Crack Tip Advancement	**Yanan Sun** (Swansea University)
212	3.9	Dynamic Analysis of a Multi-Contact Problem Using Simplified Models to Study of the Influence of Clearances on Contact Forces	**Victor BLANC** (French Atomic and Alternatives Energies Commission)
215	2.8	Two-scale phase field modeling of damge and fracture for disordered media	**Ye Feng** (Tongji University)
216	3.17	The Refined Algrithm of Generalized Probability Density Evolution Equation Based on Reproducing Kernel Particle Method	**Dan Wang** (Tongji University)
218	1.23	Data-Drive Approaches in Predicting Premixed Reactive Flow	**Mohsen Ayoobi** (Wayne State University)
219	2.27	Comparisons of direct numerical simulation and penalized models to compute the flow in a porous-fluid system	**Charles-Henri C.H. Bruneau** (University of Bordeaux)
220	1.20	Machine Learning-based Approach for Predicting Defects under Uncertainty in Sheet Metal Forming Processes	**Pedro Prates** (University of Coimbra)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
222	2.25	Quantified Relationship between Properties of Fresh Self-compacting Concrete and Workability Test Performance	**Sizeng You** (Swansea University)
223	1.27	Robust Flame Frequency Response Identification via a Multi-Fidelity Approach	**Shuai Guo** (Technical University Munich)
221	1.11	On the universality of the Strouhal law for High Reynolds number bluff bodies with flow control	**Avraham Seifert** (Tel Aviv University)*
224	3.6	Numerical modelling of the uncertainties in hip prosthesis material parameters	**Abdelkhalak El Hami** (INSA Rouen)
226	1.22	Multi-scale Numerical Simulation of Reinforced Concrete Framed Structure	**Xiangling Gao** (Tongji Universiry)
227	2.21	Multiscale Moddeling of Self-Affine Rough Contact	**António M Couto Carneiro** (INEGI); (Faculty of Engineering University of Porto);
228	2.24	Multi-scale adaptive unstructured mesh predictive modelling for environmental problems	**Fangxin Fang** (Imperial College London)*
229	2.17	A Global-Local Zooming Technique	**Matthias Birner** (Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
230	**1.10**	Multiscale prediction of powder properties during pressure-assisted sintering	**Szymon Nosewicz** (Institute of Fundamental Technological Research of the Polish Academy of Sciences)
231	**1.9**	Virtual material characteriazation across scales and physics: case studies	**Anna Matveeva** (Siemens Industry Software NV)
232	**2.11**	Heat transfer partitioning models for nucleate boiling	**Robin Kamenicky** (University of Strathclyde)*
233	**2.19**	A fully coupled electromagnetic-thermal-transient mechanical simulation of the load suffered by aeronautical composite panels during lightning strikes	**Christine Espinosa** (Institut Clément Ader)
234	**1.18**	Modelling of shear bands in fluid saturated poroplastic solids with embedded strong discontinuities	**Mijo Nikolic** (University of Split)
235	**1.29**	Comparison of Two New Methods for Fatigue Reliability Analysis	**Ruofan Gao** (Tongji University)
236	**2.16**	Construction of optimal basis functions in the Partition of Unity Method and their verification in complex simulations	**Denis Düsseldorf** (University Of Bonn)
238	**3.15 (presented by:**	Metamodels for RBDO of wire bonding in microsystem packages	**Abdelkhalak El HAMI** (INSA Rouen)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
	Abdelkhalak El Hami)		
241	**1.24**	New Method for Numerical Calibration of a Rotary Kiln Model - A Multiscale Approach	**Christian Jordan** (TU Wien/Institute of Chemical Engineering)
242	**1.21**	Nanoscience applied to oil and gas technologies: a multiscale computational approach	**Caetano R Miranda** (Universidade de Sao Paulo)
243	**2.18**	Designing phononic crystal with anticipated band structure through a deep learning based data-driven method	**Zhanli Liu** (Tsinghua University)
244	**2.1**	Stochastic Finite Element Analysis of U-Shaped RC Shear Wall with a Novel Random Field Modeling Strategy for Open Thin-Walled Structural Members	**De-Cheng Feng** (Southeast University)
247	**3.7**	A Turbulence Based Sensitivity Study on Drag Prediction of the NASA Common Research Model Aircraft	**Sule Ozturk** (Istanbul Technical University)
246	**1.17**	Increased Modelling Demands by Moving from Resolved to Unresolved Simulation of Heterogeneous Reactive Systems	**Bahram Haddadi Sisakht** (TU Wien))

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
250	1.8	Assessment of the Size of the Representative Volume Element of Random Heterogeneous Materials	**Pawel Holobut** (Institute of Fundamental Technological Research, Polish Academy of Sciences)
248	2.5	Approximation of frequency response functions with the multi-element generalised polynomial chaos method	**Prem Ratan Mohan Ram** (TU Braunschweig)*; Ulrich Roemer (TU Braunschweig)
251	3.19	Scaling procedure for the design of a validation experiment on an accidental gas release	**Alberto Moscatello** (Politecnico di Torino)
237	2.4	A Vibrational study of graphene sheets, carbon nanotubes, and nanocones	**Reza Ghaffari** (Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University)
252	3.10	A DFT study of single layer blue phosphorus and its implementation in a continuum model	**Farzad Shirazian** (Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University)
253	2.9	A Fully Second-Order Homogenisation Model for the Analysis of Multi-Phase Materials at Finite Strains	**Igor André Rodrigues Lopes** (Faculty of Engineering University of Porto)
254	3.14	Ductile failure analysis in metallic materials through computational homogenisation	**Rui Coelho** (Faculty of Engineering University of Porto)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
255	**3.5**	Computational Aspects on the Constitutive Modelling of Multiphase Alloys	**Miguel V Carvalho** (Faculty of Engineering of the University of Porto)
256	**2.3**	A Finite-Strain Elasto-Viscoplastic Model for Rubber Toughened Glassy Polymers: Formulation and Validation	**Bernardo Proença Ferreira** (Faculty of Engineering University of Porto)
259	**3.8**	PGD based domain decomposition method applied to parameterized seismic models	**Prattya Datta** (BSC)
261	**2.14**	Fully coupled multi-scale finite element analysis of TRIP-assisted multi-phase alloys	**Daniel de Bortoli** (Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI)
249	**3.18**	Optimization of Control Parameters for an Electrified Vertical Take-off Landing Vehicle Using the Integral Squared Method	**Ibrahim Cicek** (Istanbul Technical University)
263	**2.23**	Multiscale stochastic simulations using a MFH model constructed from full-field SVE realizations	**Juan Manuel Calleja** (ULiege)
264	**2.2**	Simulation of adhesive squeeze flow using smoothed particle hydrodynamics	**Lorraine Aparecida Silv**a (Institut Clément Ader)
262	**2.12**	Computational methods for hybrid multiscale modelling in immunology	**Dmitry Grebennikov** (MIPT);

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
265	2.19	A Thermo-Mechanically Coupled Cutting Simulation of Ti-6Al-4V Using Advanced Meshless Methods	**Mohamadreza MA Afrasiabi** (ETH Zurich)
266	2.10	Multiphysics Simulation of Laser Metal Deposition Manufacturing Process Using a Meshless Method	**Boussad Abbès** (University of Reims Champagne-Ardenne)
267	3.4	Micromechanical Modeling and Estimation of Elastic Properties of Pure MXene (Ti3C2Tx) Films	**Shreyas Srivatsa** (AGH University of Science and Technology)
268	2.22	Computational study of deformation mechanisms in hcp metal: Application to pure zinc	**Fazilay ABBES** (University of Reims Champagne Ardenne)
269	2.7	Multiphysical simulation of aluminum panels' behaviour hit by lightning strikes	**Florent Grotto** (ICA)
270	2.13	Modelling of honeycomb composite sandwich panel with flax fiber skin	**Matteo Riganti** (ISAE-SUPAERO)
271	3.12	Presented by Abdelkhalak El HAMI: Probablistic approach of a dynamic analysis of wind turbine on flexible foundation	**Abderraouf KAMEL** (INSA Rouen)
213	1.25	A phase-field damage model with micro inertial effect for dynamic failure of quasi-brittle materials	**Lu Hai** (Tongji University);
273	2.30	Multi-scale Reliability Based Design Optimisation for	**Sadik L. Omairey** (University of Aberdeen);

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
		Unidirectional FRP Composite Laminates	
204	**2.15**	New Vortex Identification Methods for Tuebulence - Omega, Liutex/Rortex, Omega-Liutex	**Chaoqun Liu** (University of TexaS AT aRLINGTON)
202	**2.29**	Examining the Mutation Effect of SLC26A4 STAS Domain By Observing the Communication Between Secondary Structures	**Sungsoo Na** Korea University
277	**2.21**	277 Performance of drag models in CFD-DEM	**Ashutosh Bhokare** (Swansea University)
276	**3.2**	276 Efficient structural reliability analysis based on polynomial chaos expansion and maximum entropy method	**Jinsheng Wang** (Swansea University)
278	**2.26**	PyEFEM: Massively parallel python based FEM framework for flow problems	**LIANG YANG** (Cranfield University)
201	**1.14**	System time-variant reliability-based structural design optimization of deteriorated truss bridges	**Younes Ya Aoues** (Normandie Université, INSA Rouen Normandie, LMN)

Pore Water State in Heated Concrete—Comparing a Numerical Model to NMR Measurements

Christoph Pohl [1], Jörg F. Unger[1]

[1]Bundesanstalt für Materialforschung und -prüfung

christoph.pohl@bam.de

Spalling of concrete structures is a serious issue for their safety. A better understanding of the pore water distribution and state during a fire is a prerequisite for numerical approaches to such problems.

Temperature-driven water transport in concrete consists of multiple phenomena, such as convection, diffusion, adsorption and dehydration. Distinguishing the different influences experimentally is difficult because typically they cannot be disentangled.

A common experimental setup approximates a one-dimensional flow, and places temperature and pressure gauges along the propagation direction [1]. For direct information about the water content inside a sample, methods such as NMR or neuron radiography are necessary.

A multiphase model for the flow in porous media based on [2] is presented, with dehydration and changes in the pore size distribution taken into consideration. NMR measurements for temperature-driven flow have been performed. The numerical and experimental results are compared for water transport at temperatures below the critical point. Since both the finite-element model and the experiment allow the distinction between adsorbed, capillary and bulk water, a more fine-grained view of the pore water state is obtained.

[1] P. Kalifa, F.-D. Menneteau and D. Quenard, "Spalling and pore pressure in HPC at high temperatures," *Cement and Concrete Research,* vol. 30, pp. 1915-1927, 2000.

[2] D. Gawin, F. Pesavento and B. A. Schrefler, "What physical phenomena can be neglected when modelling concrete at high temperature? A comparative study. Part 1: Physical phenomena and mathematical model," *International Journal of Solids and Structures,* vol. 48, p. 1927–1944, Jun 2011.

Computationally efficient homogenization for modeling of nonlinear functionally graded materials

Witold Ogierman [1]

[1]Silesian University of Technology, Gliwice, Poland

witold.ogierman@polsl.pl

Advanced composite materials such as functionally graded particle reinforced composites can provide unique properties due to spatially varied microstructural features. In this case prescribed properties of structural elements can be achieved for example by controlling the spatial distribution of the reinforcement. Design of such materials and prediction of their effective properties can be performed by using advanced computational methods. The present investigation is devoted to development of computationally efficient homogenization procedure for modeling of particle reinforced functionally graded materials (FGM) that exhibit elastic-plastic properties. At the macroscopic level the FGM can be regarded as material consisting of multiple layers with different volume fraction of the reinforcement [1]. The material properties of the layers can be determined in terms of microstructural features like the reinforcement volume fraction, shape etc. by using the homogenization procedure. One of the most widely used and versatile method of homogenization is based on finite element (FE) analysis of representative volume element (RVE). The FE based homogenization can be applied in modelling of nonlinear constitutive behavior and microstructures of complex geometry however in such cases it typically requires time consuming computations [2]. Moreover generation of different RVEs for different layers and usage of strongly coupled multi-scale FE^2 framework could lead to prohibitive time of computations. The other way is to use the mean field homogenization approaches among which the most popular is the Mori-Tanaka (M-T) method which provides good predictive capabilities and low computational cost. On the other hand the M-T method is limited to the case of the ellipsoidal shape of the reinforcement only for which the fundamental Eshelby's solution is valid [3]. In addition, methods of isotropic approximation of tangent stiffness tensor are required in order to achieve a reasonable accuracy for elastic-plastic materials. Nevertheless, these limitations can be overcome by using numerical solution of the single

inclusion problem instead of using Eshelby's fundamental solution [4, 5]. Generally, such a hybrid M-T/FE method is more versatile than analytical M-T method and provide more time-efficient solution than pure FE method. The present study is devoted to application of novel simplified homogenization method for modeling of elastic-plastic FGMs based on the hybrid M-T/FE. The idea is to obtain the nonlinear mean field relation between the macroscopic strain and the strain in the reinforcement by solving the Eshelby's problem numerically only once and then approximate the properties of layers containing different volume fractions of the reinforcement analytically. This approach may lead to achieve very time-efficient solution while simultaneously providing high accuracy.

The presentation will cover mainly: details of the numerical procedures connected with the novel homogenization method, discussion on accuracy of proposed method both in linear-elastic and nonlinear regime, comparison of the obtained results with the results of homogenization based on finite element (FE) analysis of the representative volume element (RVE) containing complex geometry, examples illustrating a potential and effectiveness of the proposed approach.

Acknowledgement

The research for this paper was financially supported by the National Science Centre, Poland (Grant No. UMO-2016/21/N/ST8/01119) and the Silesian University of Technology (Grant No. 10/040/RGJ19/0081).

References

1. Schmauder, S., Weber, U. Modelling of functionally graded materials by numerical homogenization, *Archive of Applied Mechanics*, 71(2), 182-192, 2001

2. Ogierman, W., Kokot, G. Generation of representative volume elements of heterogeneous materials with distributed orientations of inclusions. *Composite Structures*, 201, 636–646, 2018.

3. Eshelby, J. D. The determination of the elastic field of an ellipsoidal inclusion, and related problems. *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, 241(1226), 376–396, 1957.

4. Brassart, L., Doghri, I., Delannay, L. Homogenization of elasto-plastic composites coupled with a nonlinear finite element analysis of the equivalent inclusion problem. *International Journal of Solids and Structures*, 47(5), 716–729, 2010.

5. Ogierman, W. Hybrid Mori-Tanaka/Finite Element Method in Homogenization of Composite Materials with Various Reinforcement Shape and Orientation, *International Journal for Multiscale Computational Engineering* (In Press), 2019.

Multiphysics Computation in Batteries Involving Electromagnetism and Thermomechanics

Bilen Emek Abali [1]

[1]Technische Universität Berlin, Institute of Mechanics, Einsteinufer 5, 10587 Berlin, Germany

bilenemek@abali.org

An electrochemical cell like a Li-ion battery has to be modeled by involving multiphysics phenomena called and studied separately. Electromagnetism is governed by Maxwell equations; thermomechanics is given by balance equations, all these equations are incompatible with each other making a derivation of the unique and consistent theory very challenging. In the case of electro-thermo-mechanical systems, we established the derivation of all necessary equations by using theoretical thermodynamics[1] and their accurate computation[2] by using a monolithic solution technique[3] based on open-source packages developed and known under the FEniCS project.[4]

This talk is on the extension of the theoretical framework for incorporating diffusion as a result of balance equations for every constituent---this approach is called the mixture theory in continuum mechanics. As a system alike Li-ion battery consolidates all possible physical phenomena in a continuum body, we need to solve coupled and nonlinear field equations in a monolithic approach. Especially in electromagnetism, there are various methods to circumvent emerging numerical problems. Hence, a strong emphasis will be put on the computation of electromagnetic fields in a robust algorithm.

[1] Abali, B. E., & Reich, F. A. (2017). Thermodynamically consistent derivation and computation of electro-thermo-mechanical systems for solid bodies. Computer Methods in Applied Mechanics and Engineering, 319, 567-595.
[2] Abali, B. E., & Reich, F. A. (2018). Verification of deforming polarized structure computation by using a closed-form solution. Continuum Mechanics and Thermodynamics, 1-16.
[3] Abali, B. E. (2017). Computational Reality: Solving Nonlinear and Coupled Problems in Continuum Mechanics. Springer Nature, Singapore.
[4] https://fenicsproject.org/

Presenting Author, Second Author, Third Author

On modeling interfaces in composite with multi-physic coupling

Michele Serpilli [1], Raffaella Rizzoni [2], Serge Dumont [3], Frédéric Lebon[4]

[1]Università Politecnica delle Marche, Ancona, Italy

m.serpilli@univpm.it

[2]Università di Ferrara, Ferrara, Italy

raffaella.rizzoni@unife.it

[3]Université de Nîmes, Nîmes, France

serge.dumont@unimes.fr

[4]Aix-Marseille Univ, CNRS, Centrale Marseille, France

lebon@lma.cnrs-mrs.fr

In the last decades, the interest in bonded structures, obtained by assembling different parts made of possibly different materials to compose a unique structure, is strongly increased. The advantage of such composites is that their mechanical performances and properties are designed to be superior to those of the constituent materials acting independently. Nowadays, composites have been more frequently used in civil, naval, aeronautical and mechanical engineering, in general. The bond among the various parts of the composite may generally be imperfect and discontinuities in physical fields can arise, significantly changing the mechanical and physical properties of the material. Hence, a correct theoretical modeling of the imperfect bonding plays an important role in engineering design.

In the present work we focus our attention to a specific type of composite, constituted by two media, called the adherents, bonded together with a thin interphase layer, called the adhesive. We assume that the composite constituents are made of different multi-physic materials with highly contrasted constitutive properties. The study considers a generic multi-physic coupling in a very general framework and can be adapted to well-known multi-physic behaviors, such as piezoelectricity, thermo-elasticity, magneto-electro-thermo-elasticity, as well as to multifield microstructural theories, such as micropolar and microstretch elasticity. The analysis has been carried out by means of asymptotic expansions method. The use of this technique spans from the justification of classical theories of thin structures [1] to the rigorous derivation of simplified models for complex assemblies, presenting thin interphases, in the field of linear elasticity [2] as well as in piezoelectricity, taking into account thermal, magnetic and other physical interactions [3,4]. The asymptotic methods allow to replace the adhesive layer with a two-dimensional surface, the so-called imperfect interface, with non-classical transmission conditions between the two adherents.

By defining a small parameter ε, associated with the thickness and constitutive properties of the middle layer, we perform an asymptotic analysis. We assume that the thickness depends linearly on ε, while the multi-physic stiffness ratios between the adherents and the adhesive depends on ε^p. We identify three critical exponents p, corresponding to different imperfect interface models: p=1, the *soft* (also called *lowly-conducting*) multi-physic interface model, for which we rescale the constitutive coefficients of the intermediate layer with ε; p=0, the *hard* (also called *moderately-conducting*) multi-physic interface model, for which the rigidities of the constituent materials have the same order of magnitude; p=-1, the *rigid* (also called *highly-conducting*) multi-physic interface model, for which we choose 1/ε as rescaling. Following the approach by [2], we derive the limit transmission problem at order zero. Moreover, taking into account higher order terms of the asymptotic expansion, namely the first corrector terms, we give a more precise approximation of the actual mechanical behavior of the interface. Finally, a general multi-physic interface model has been developed, including the three aforementioned limit behaviors, and numerically tested through the finite element method. In particular, in the framework of piezoelectricity, we compare the results obtained by modeling the adhesive as an interphase, having a thin finite thickness, with the results obtained with the general multi-physic interface model.

References.

[1] Ciarlet PG Mathematical Elasticity, vol. II: Theory of Plates. North-Holland, Amsterdam, 1997.
[2] Rizzoni R, Dumont S, Lebon F, Sacco E (2014) Higher order models for soft and hard elastic interfaces. Int. J. Solids Struct. 51(23-24): 4137-4148.
[3] Serpilli M (2015) Mathematical modeling of weak and strong piezoelectric interfaces, J. Elasticity 121(2): 235-254.
[4] Serpilli M (2017) Asymptotic interface models in magneto-electro-thermo-elastic composites. Meccanica 52(6): 1407-1424.

Sub-Modeling Approach to Investigate the Cracking Behavior of Reinforced Concrete Structures Considering Polymorphic Uncertainty

Katharina Kremer [1] , Philipp Edler [1], Steffen Freitag [2], Günther Meschke [1]

[1] Ruhr University Bochum, Germany
{katharina.kremer, philipp.edler, guenther.meschke}@rub.de

[2] Ruhr University Bochum, Germany
steffen.freitag@sd.rub.de

The cracking behavior of reinforced concrete (RC) structures is influenced, beyond temperature and loading, by the reinforcement design and the bond characteristics between the steel reinforcement and the concrete. In this contribution, a RC two-span beam subjected to its self-weight and a traffic load, is investigated regarding the crack pattern and the evaluation of crack widths, considering uncertainties of material data. A sub-modeling approach is used for investigating only highly stressed parts of the structure with a detailed model taking the boundary conditions from a coarse structural model into account to reduce the computation time. In a first step, the RC beam is analyzed with a continuum damage model to identify the critical sections ("hot spots"), where cracks are expected to appear. In the next step, the identified hot spots are analyzed with a more refined model enabling a discrete representation of cracks via cohesive interface elements [1]. In both models, the reinforcement is considered by means of a discretization independent embedded rebar model, where frictional contact between steel reinforcement and concrete is taken into account to consider the tension stiffening [2].

The main factors, which influence the cracking behavior (onset of cracking and crack width) of RC structures, are the tensile strength, the Young's modulus and the concrete-steel bond characteristics. These parameters are considered as uncertain parameters within the simulation. In general, aleatoric uncertain parameters, which are concerned with randomness, are quantified by stochastic distributions and epistemic uncertain parameters, which deal with lack of knowledge, are quantified by intervals or fuzzy numbers. In this contribution, the Young's modulus, which is assumed as fully correlated to the concrete strength according to fib Model Code [3], is considered as a stochastic parameter, which is lognormal distributed. The traffic load is also described by a stochastic parameter, using a Gaussian distribution. For investigating the influence of

imprecise rebar bond behavior to the cracking behavior, the bond strength is considered as an epistemic uncertain parameter. In the fib Model Code [3] the maximal bond strength τ_{max} is proposed as a function of the compressive strength. This value is taken as a reference value, to quantify the interval bounds for the bond strength.

In a first investigation [4] the influence of the polymorphic uncertain parameters was already investigated for a 2D Finite Element (FE) simulation with chosen reinforcement of five rebars with a diameter of 20 mm for the lower and upper reinforcement layers based on a classical reinforcement design. It was found, that for a fixed Young's modulus of concrete the lower and upper bound of the bond strength has almost no influence to the load-displacement curve for the full structural model, but the comparison of the crack pattern of the sub-models for the lower and upper bound of the bond strength shows significant difference in crack widths and crack patterns, which, in turn, affects the durability of the structure. In this contribution, results from a 3D simulation of the RC beam using polymorphic uncertain parameters are presented. Here, the focus will be on the influence of the reinforcement design (smaller vs. larger diameters with same area of reinforcement), considering uncertain bond strength, on the distribution of the crack pattern and crack widths, respectively.

References

[1] Zhan, Y.; Meschke, G.: Multilevel computational model for failure analysis of steel-fiber-reinforced concrete structures. Journal of Engineering Mechanics (ASCE), 142, 2016, pp. 1-14.

[2] Gall, V. E.; Butt, S.; Neu, G.; Meschke: An embedded rebar model for computational analysis of reinforced concrete structures with applications to longitudinal joints in precast tunnel lining segments. In: G. Meschke, G.; Pichler, B.; Rots, J. G. (Eds.), Computational Modelling of Concrete Structures (EURO-C 2018), CRC press, 2018, pp. 705-714.

[3] International Federation for Structural Concrete CEB-FIP Model Code 1990 (Design Code), Thom, 1993.

[4] Kremer, K.; Edler, P.; Miska, N.; Leichsenring, F.; Balzani, D.; Freitag, S.; Graf, W.; Kaliske, M.; Meschke, G.: Modeling of structures with polymorphic uncertainties at different length scales. Surveys for Applied Mathematics and Mechanics (GAMM-Mitteilungen), 2019, accepted.

A computational multi-physics model to predict The chemo-mechanical degradation of historical oil paintings

Emanuela Bosco [1], Gijs J.A.M. Eumelen [1], Akke S.J. Suiker [1]

[1]Eindhoven University of Technology, The Netherlands

e.bosco@tue.nl

A common, yet critical degradation mechanism in historical oil paintings is related to the formation and growth of metal soap crystals. Historical oil paintings typically consist of layers of a drying oil binding medium that contains metal-based pigment particles. The chemical reaction between the metal ions present in the pigments and the saturated fatty acids released by oil binder results in the formation of metal soaps, which can crystallize and grow into large protrusions [1]. This originates mechanical strains in the system, deforming paint layers and ultimately leading to cracking, flaking and delamination of the paint. This work presents a computational multi-physics framework to predict the degradation of historical oil paintings induced by metal soap formation and growth. The chemical processes are described through a diffusion-reaction model [2] formulated by taking the saturated fatty acids as the reference diffusing species. The reaction term allows to represent the formation and growth of a metal soap crystal. A chemically-induced growth strain introduces the coupling between the chemical and the mechanical models, by quantifying the effect of metal soap growth on the stress field generated in the paint system. Further, the change in mechanical properties associated to the formation of crystalline metal soap is described through a rule of mixtures based on the volume fractions of formed metal soap and the original oil binder material. The proposed model is implemented within a finite element setting, combined with a discrete crack approach, for which cohesive interface elements are placed between all continuum elements discretizing the paint layer geometry. The nucleation and propagation of cracks is prescribed according the interface damage model proposed in [3]. Furthermore, across crack faces, the constitutive relation between the flux and the concentration of saturated fatty acid is given as a function of mechanical damage. The numerical update procedure of the coupled chemo-mechanical processes is performed by using a staggered scheme. A set of numerical simulations illustrates the capability of the model to predict metal soap

crystallization and growth and the fracture induced in the paint. The study finally illustrates the influence of different chemical and mechanical parameters (elastic stiffness mismatch between the paint and the metal soap crystal, chemical growth strain and reaction rate) on the chemo-mechanical degradation of the paint layer.

References

[1] J. J. Hermans, K. Keune, A. van Loon, P. D. Iedema, An infrared spectroscopic study of the nature of zinc carboxylates in oil paintings, Journal of Analytical Atomic Spectrometry 30 (7) (2015) 1600-1608.

[2] T. S. Hille, S. Turteltaub, A. S. J. Suiker, Oxide growth and damage evolution in thermal barrier coatings, Engineering Fracture Mechanics 78 (10) (2011) 2139-2152.

[3] M. V. Cid Alfaro, A. S. J. Suiker, R. de Borst, J. J. C. Remmers, Analysis of fracture and delamination in laminates using 3D numerical modelling, Engineering Fracture Mechanics 76 (6) (2009) 761-780.

A coupled chemo-mechanical model for biogenic Sulfide corrosion in concrete sewer pipes

Emanuela Bosco [1], Frits A.M. Rooyackers[1], Akke S.J. Suiker [1], Francois H.L.R. Clemens[2,3]

[1]Eindhoven University of Technology, The Netherlands

[2]Delft University of Technology, The Netherlands

[3]Deltares,The Netherlands

e.bosco@tue.nl

Durability of concrete is a relevant issue in the structural design of sewer systems, which largely impacts the maintenance and rehabilitation costs associated to the sewerage infrastructure. In this context, chemical attacks by sulfates, and in particular biogenic sulfide corrosion, are primary causes of concrete degradation. Biogenic sulfide corrosion is caused by Thio-oxidans bacteria, which may grow on the surface of concrete above the wastewater level in relative acidic environments. These bacteria are able to oxidize sulfur compounds into sulfuric acid that may diffuse into the concrete pipe, reacting with calcium hydroxide to form gypsum and ettringite [1]. These newly formed compounds have only limited structural properties. Additionally, they occupy a larger volume than the original material, introducing an expansive strain that can result in the cracking of concrete and in the loss of aggregates. Conversely, cracking phenomena influence the diffusivity of the system, thus further promoting the ingress of sulfuric acid and accelerating concrete degradation.

This contribution precisely proposes a coupled chemo-mechanical model to predict biochemical degradation of concrete sewer pipes. While some recent works in the literature deal with the numerical simulation of the biochemical degradation process by mainly considering ettringite formation [2, 3], this study focuses on the process of gypsum formation. The chemical model accounts for several (diffusion-) reaction equations, coupled by their reaction terms. A chemical strain, defined as a function of gypsum concentration, allows to represent the expansive nature of gypsum. Further, the governing constitutive equations are formulated as a function of chemical and mechanical damage parameters, which account for the effects of chemical and mechanical degradation. The

model is implemented within the finite element framework. A series of numerical simulations is performed on a sewer pipe geometry, providing the concentration evolutions of the relevant chemical species in the system and demonstrating the capability of the model to adequately estimate the development of damage.

References

[1] Davis, J., Nica, D., Shields, K., & Roberts, D. (1998). Analysis of concrete from corroded sewer pipe. International Biodeterioration & Biodegradation, 42, 75–84.

[2] Idiart, A., Lopez, C., & Carol, I. (2010). Chemo-mechanical analysis of concrete cracking and degradation due to external sulfate attack: A meso-scale model. Cement and Concrete Composites, 33, 411–423.

[3] Cefis, N., & Comi, C. (2017). Chemo-mechanical modelling of the external sulfate attack in concrete. Cement and Concrete Research, 93, 57–70.

Degradation of Lithium-Ion Batteries in Aerospace

Linda J. Bolay[1,2], Birger Horstmann[1,2], Omar S. Mendoza-Hernandez[4], Yoshitsugu Sone[4,5], Arnulf Latz[1,2,3]

[1] Institute of Engineering Thermodynamics, German Aerospace Center, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany

[2] Helmholtz Institute Ulm for Electrochemical Energy Storage, Helmholtzstrasse 11, 89081 Ulm, Germany

[3] Institute of Electrochemistry, University of Ulm, Helmholtzstrasse 11, 89081 Ulm, Germany

[4] Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency, 3-1-1 Yoshinodai, Chuo-ku, Sagamihara, Kanagawa, 252-5210 Japan

[5] The Graduate University of Advanced Studies (SOKENDAI), 3-1-1 Yoshinodai, Chuo-ku, Sagamihara, Kanagawa, 252-5210 Japan

linda.bolay@dlr.de

Lithium-ion batteries are the technology of choice for a broad range of applications due to their performance and long-term stability. The performance and durability of lithium-ion batteries is heavily impacted by various degradation mechanisms. These include the growth of the solid-electrolyte interphase (SEI) and the deposition of metallic lithium on the surface of the negative electrode, referred to as lithium plating. Long-term SEI growth is the biggest contributor to capacity fade in lithium-ion batteries. Lithium plating, which occurs in low temperature or high current charging, can result in capacity fade or even thermal runaway.

In our group we develop multiphysical models and perform simulations for various types of batteries. In order to describe the internal processes of Li-ion batteries, we derive thermodynamic consistent transport theories [1]. Based on these, our group has developed models for long-term SEI growth [2,3] and for lithium plating in 3D electrode microstructures [4].

Such models predict battery performance over short time scales during single charging and discharging as well as battery degradation over long time scales during continued cycling.

Finally, we want to understand the processes taking place in Li-ion batteries and observe them during battery operation. Here, we discuss perfomance and lifetime for the batteries of in-orbit satellite REIMEI [5]. To this end, we parameterize our model by comparing the electrochemical simulations to various experimental and in-flight data. By incorporating our new model for continued growth of the SEI [2], we simulate degradation in micro-structured electrodes in one and three dimensions. We are the first to understand experimentally observed inhomogeneities in the SEIs thickness throughout the negative electrode. Furthermore, our degradation model applies to battery storage as well as to battery cycling. We will further discuss lithium plating and perform state estimation of the REIMEI battery to predict its state-of-health in earth orbit.

References:

[1] A. Latz, J. Zausch, Beilstein Journal of Nanotechnology 6 (2015) 987, doi:10.3762/bjnano.6.102.

[2] F. Single, A. Latz, B. Horstmann, ChemSusChem 11(12) (2018) 1950-1955, doi: 10.1149/2.0121711jes.

[3] F. Single, B. Horstmann, A. Latz, Journal of The Electrochemical Society 164(11) (2017) E3132-E3145. doi:10.1149/2.0121711jes.

[4] S. Hein, A. Latz, Electrochimica Acta 201 (2016) 354-365, doi: 10.1016/j.electacta.2016.01.220.

[5] M. Uno, K. Ogawa, Y. Takeda, Y. Sone, K. Tanaka, M. Mita, H. Saito, Journal of Power Sources 196(20) (2011) 8755-8763, doi:10.1016/j.jpowsour.2011.06.051.

Reduced-order Modelling Scheme for Problems with Fully Resolved Microstructures Generated by Generalized Periodic Unit Cells

Martin Doškář [1], Jan Novák [1], and Jan Zeman [1]

[1]Czech Technical University in Prague

martin.doskar@fsv.cvut.cz

Microstructural details influence the performance of products especially when it comes to localizing phenomena and problems with low separation of microstructural and macroscopic scales. However, hardly ever the actual microstructural composition within a macroscopic product is a-priori known, thus a statistical quantification of product responses under varying microstructural realizations is desired. This may require (i) procedures for generating random yet statistically coherent realizations of a given microstructure and (ii) efficient numerical schemes for related analyses.

Addressing the first requirement, we have proposed a representation of material microstructures built on the formalism of Wang tiles (Novák et al., 2012). Our approach delivers a compromise between the (Statistically Equivalent) Periodic Unit Cell characterization of material microstructures and an approach in which stochastic microstructural realizations are generated each time anew (e.g. using costly optimization approaches). With only a handful of small microstructural cells – Wang tiles – with predefined mutual compatibility arbitrarily large, stochastic microstructural samples can be generating following a simple stochastic assembly algorithm. In our previous works, only the geometrical part of the tile-based representation has been utilised, e.g. (Doškář et al., 2018). However, given the repeating occurrence of individual tiles in the assembled microstructural realizations, the tile-based representation holds promise also for addressing the second requirement.

In this contribution, we present a numerical scheme that combines the eXtended Finite Element Method (XFEM) and Reduced Order Modelling (ROM) to accelerate numerical analyses of macroscopic problems whose microstructural geometry was generated by means of Wang tiles. The scheme comprises two ingredients. First, inspired by numerical homogenization, we extract characteristic fluctuation responses of the microstructure at the level of the compressed tile representation. Second, we combine

a coarse finite element discretization (unaware of the underlying microstructure) of a macroscopic problem and the assembled characteristic fluctuations using an XFEM ansatz. While the macroscopic discretization captures the global character of a macroscopic response, the XFEM ansatz serves as an interpolation between assembled fluctuation modes, which were derived without any knowledge of the shape or loading of the macroscopic problem. The scheme thus differs from standard ROM approaches as we don't sample a parametric space and extract response of the macroscopic problem; in this sense, it resembles more the XFEM formulations with dictionary solutions, e.g. (Strouboulis et al., 2003). On the other hand, we adopt the ROM perspective in implementation due to its straightforward way of posing Dirichlet boundary conditions and potential for additional acceleration by means of hyper-reduction methods.

Acknowledgement

This work was partially funded by the Ministry of Industry and Trade of the Czech Republic through the project No. FV10202. In addition, MD and JN acknowledge the financial support through OP VVV projects International Mobility of Researchers Nos. CZ.02.2.69/0.0/0.0/16_027/0008465 and CZ.02.2.69/0.0/0.0/17_050/0008025.

References

Doškář, M., Zeman, J., Jarušková, D., Novák, J., 2018. Wang tiling aided statistical determination of the Representative Volume Element size of random heterogeneous materials. European Journal of Mechanics - A/Solids 70, 280–295. https://doi.org/10.1016/j.euromechsol.2017.12.002

Novák, J., Kučerová, A., Zeman, J., 2012. Compressing random microstructures via stochastic Wang tilings. Physical Review E 86, 040104(R). https://doi.org/10.1103/PhysRevE.86.040104

Strouboulis, T., Zhang, L., Babuška, I., 2003. Generalized finite element method using mesh-based handbooks: application to problems in domains with many voids. Computer Methods in Applied Mechanics and Engineering 192, 3109–3161. https://doi.org/10.1016/S0045-7825(03)00347-5

Fragment size characterization for granular flow in highly damaged ceramics

Lori Graham-Brady [1], Amartya Bhattacharjee [1]

[1]Johns Hopkins University

lori@jhu.edu

Granular mechanics has been studied extensively, particularly in the field of geomechanics. However, the onset of granular mechanics and flow characteristics in a dense comminuted brittle material is still not well understood. We know that the initial grain size distribution plays an important role in determining granular flow characteristics. Under brittle dynamic compression loading, as often observed in impact experiments, wing crack- growth from pre-existing defects, subsequent crack interactions and coalescence mechanisms lead to fragmentation and granular flow in highly damaged regions. This talk focusses on determining an approximate initial fragment size distribution for granular flow and can be used in general, to obtain fragment size statistics from crack size statistics. Crack populations have been numerically simulated from a known distribution on effective length and orientation of cracks, and later stage coalescence has been accounted for by using a threshold distance around a crack tip. Fragment statistics, like size and shape distribution have been obtained by using a connected region-based algorithm. The same approach has been extrapolated in three dimensions, but here the cracks have been simulated as elliptical cracks with a thick ring around the edges. The ring size accounts for the threshold coalescence distance, and is obtained using crack-bridge strength calculations. Fragments, as before, are obtained as connected regions, and then allowed to dilate till they fill up the space. Preliminary investigation hints at a power law based distribution for fragment sizes. Although the particular problem has been set to obtain fragment size statistics from prior information about cracks, they can also be used to obtain a general fragmentation criterion.

Development of a modified Voronoi's tesselation algorithm for the determination of the effective properties of cork-based composites

Marco Delucia [1], Anita Catapano [2], Marco Montemurro [1], Jérôme Pailhès [1]

[1] Laboratoire I2M, CNRS UMR 5295, Arts et Métiers ParisTech, 33400 Talence (France)

marco.delucia@ensam.eu, marco.montemurro@ensam.eu and jerome.pailhes@ensam.eu

[2] Laboratoire I2M, CNRS UMR 5295, Bordeaux INP, Université de Bordeaux, 33400 Talence (France)

anita.catapano@bordeaux-inp.fr

Cork is a natural, recyclable and biodegradable industrially useful material with remarkable properties as lightness, excellent thermal and sound insulating properties mainly due to its honeycomb-like microstructure. Cork is extracted periodically, in a sustainable manner, from the outer bark of *Quercus Suber L.* and, depending on the type of final product, it can be exploited directly in its natural form or it can be used as cork-based agglomerate or composite [1] wherein the cork granules are mixed with a polymeric binder.

The mesostructure of cork agglomerates is characterized by randomly distributed polygonal particles which, combined with the complex microstructure of the cork, leads to complex stress/strain distributions and damage mechanisms. Omitting the effects of the honeycomb microstructure of the cork, macroscopic thermal and elastic behaviour of cork-based agglomerates depends upon different parameters defining the mesoscopic representative volume element (RVE) of the agglomerate: spatial orientation and shape of the grains, material properties of matrix and cork (including anisotropy of cork) as well as their volume fraction, percentage of voids and the matrix/grain interface properties [2,3].

The aim of the present work is to propose a general multi-scale numerical homogenisation procedure capable of determining the effective thermal and elastic properties of cork-based agglomerates. The fundamental aspect on which the proposed work is focused consists in generating a realistic mesostructural geometry of the cork-based composite. More precisely, a 2D as well a 3D parametric computational model based on a modified Voronoi’s tessellation algorithm has been developed and the strain

energy homogenisation technique for heterogeneous media [4] has been used for determining the effective properties of the agglomerate at the macroscale level. In this new algorithm for mesostructure generation, several aspects of fundamental importance have been taken into account:

- the polygonal shape of cork particles that show sharp angles, convexities and concavities;
- the transversely isotropic mechanical behavior of cork, whose material frame is randomly oriented within the mesostructured;
- the random geometrical orientation of cork particles;
- the high variability of cork mechanical properties;
- the variability of porosity distribution.

All these aspects have been considered in the development of the algorithm which has been coded in Python environment.

The 2D and 3D artificial mesostructures have been utilized to perform the strain-energy based homogenisation of elastic and thermal properties of different cork-based composites and the Monte Carlo method has been used to take into account the variability of the parameters at the mesoscale on the equivalent thermo-elastic behaviour at the macroscopic scale.

Numerical results have been compared firstly to the numerical ones obtained on mesostructures achieved by means of the digital image correlation (DIC) technique and then to the experimental ones in order to show the effectiveness of the proposed procedure.

[1] H. Pereira, *Cork: Biology, Production and Uses*, 2007.

[2] P. T. Santos, S. Pinto, P. A.A.P. Marques, A. B. Pereira, and R. J. Alves de Sousa. *Agglomerated cork: A way to tailor its mechanical properties*. Composite Structures, 178:277-287, 2017.

[3] P. T. Santos, J. S. Amaral, V. A. F. Costa, and V. S. Amaral. *Thermal Conductivity of Agglomerate Cork*. In Materials Research Proceedings, Volume 3, 1-10, 2017.

[4] E. J. Barbero. *Finite element analysis of composite materials using ansys*. 2013.

Data driven computational analysis of open foam materials

Nanda Gopala Kilingar[1], Ludovic Noels[1], Thierry J. Massart[2]

[1]Université de Liège (ULiège)

ngkilingar@uliege.be

[2]Université Libre de Bruxelles (ULB)

An automated approach, that relies on the use of distance and level set functions as explained in [1], has been described in [2] to build computationally Representative Volume Elements (RVE) of open foam materials, enabling the study of the effects of the microstructural features on the macroscopic behavior. These models have been compared with real foam samples from existing literature to verify statistically the morphological properties like face-to-cell ratio, edge-to-face ratio and strut length distribution along with the variations in the strut morphology like the shape of cross-sections of the struts and their variation along the axis of the struts. The responses obtained from a uniaxial compression test of the sample RVEs have been validated against the experimental observations and the results have showed close similarity with respect to the variations in the foam density. This approach enables us to generate multiple Stochastic volume elements (SVE) and get their material response in a short period of time.

In [3], the authors have taken inspiration from artificial neural network concepts and used linear elastic RVE data to train a material network to describe complex material

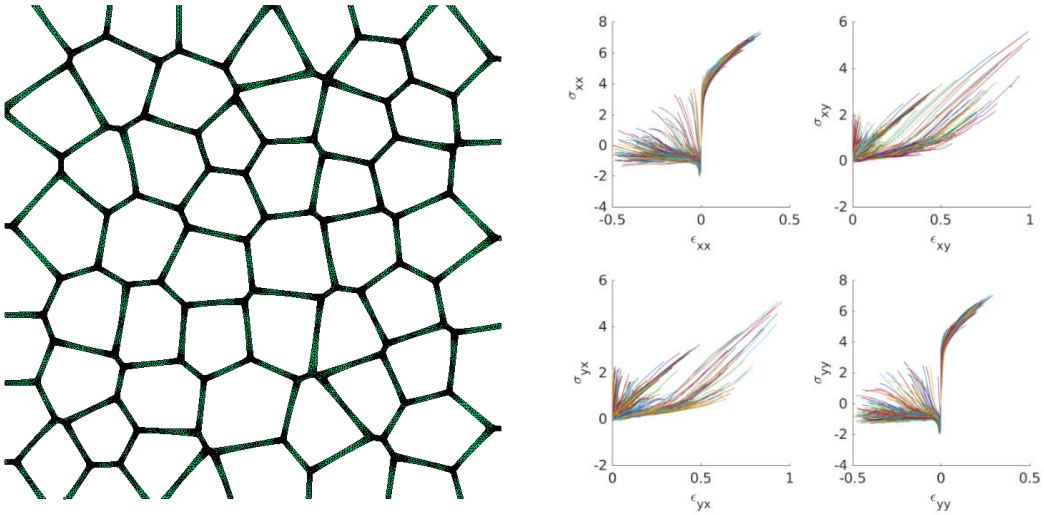


Figure 1 A 2D RVE of an open foam and its response to various deformation loads

behavior. They have also validated the extrapolations of the trained network to a wide range of problems, including non-linear history-dependent plasticity and finite-strain hyper-elasticity under large deformations.

In the current work, the goal is to utilize the material responses obtained from the SVEs as the prespecified material data set (Figure 1) and investigate the performance of various data-driven solvers on these data sets in order to eliminate the experimental testing altogether with the knowledge that the material response is in close agreement to that of the RVEs.

References

[1] B. Sonon, B. Francois and T. J. Massart, "An advanced approach for the generation of complex cellular representative volume elements using distance fields and level sets," *Computational Mechanics*, 2015.

[2] N. G. Kilingar, K. Ehab Moustaa Kamel, B. Sonon, T. J. Massart and L. Noels, "Computational generation of open-foam representative volume elements with morphological control using distance fields," *Under review*.

[3] Z. Liu, C. T. Wu and M. Koishi, "A Deep Material Network for Multiscale Topology Learning and Accelerated Nonlinear Modeling of Heterogeneous Materials," *Computer methods in applied mechanics and engineering*, 2018.

Simulation Model for Single unit Warpage of Shadow moire in Flip-Chip Process

Wan-Chun Chuang [1,2*], Wei-Long Chen [1]

[1] Department of Mechanical and Electro-Mechanical Engineering, National Sun Yat-sen University, Kaohsiung, Taiwan, R.O.C.

[2] Department of Sports Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan, R.O.C.

wcchuang@mail.nsysu.edu.tw

Background

The demand for lightweight and high functionality devices is always in the development of the smaller and lighter package technology so that Flip-Chip and Wafer-Level package technology develop. In 2018 S. J. Oon [1] mentioned that because of the CTE(Coefficient of Thermal Expansion) mismatch of the materials, thus, the package structure will occur warpage in a heating process such as Shadow moire. Worst of all, warpage will result in low yields on the production line.

Research Methods

The research process comprised two steps: 1) setup simulation model and boundary condition, 2) setup material parameter. (1)Simulation model and boundary conditions: COMSOL Multiphysics simulation software was used to establish single unit simulation model. The geometry of model as follows: PKG was 7*7*0.45 mm^3, die was 6.3*6.34*0.23 mm^3, bump pitch was 0.19 mm, and solder ball diameter was 0.25 mm. The boundary condition was set as scroll between the end of the single unit model and the ground. Besides, the temperature was 25°C →260°C→25°C and process time was 1100s for shadow moire measurement. (2) Material parameter: Tables 1 list the material parameters settings of the bump, silicon and substrate. All the materials were isotropic in this study. However, the properties of the compound were easily affected by temperature. Therefore, the compound was measured with DMA(Dynamic Mechanical Analysis) and TMA(Thermomechanical Analysis) at different temperatures, Fig. 1 illustrates the Young's modulus and CTE of compound.

Tables 1: Material parameters of the bump, silicon and substrate

	Bump SAC405	**Silicon<100> (Die)**	**Substrate**
Young's modulus (GPa)	53	131	26 (25°C),15 (260°C)
Poisson's ratio	0.40805	0.27	0.2
Density (kg/m^3)	7445.45	2330	1938

CTE(ppm/°C)	20	2.8	15 (25°C),6 (260°C)

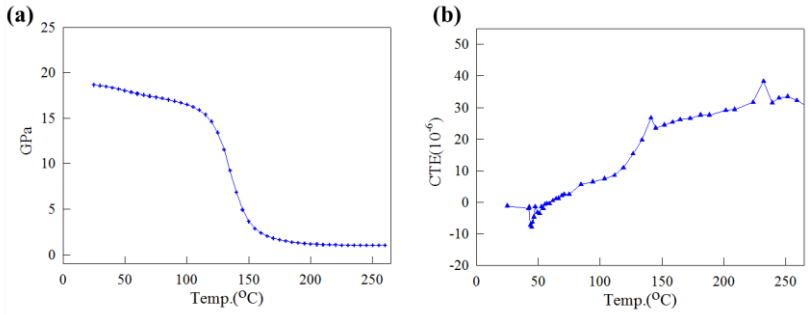


Fig. 1: Material parameters of compound at different temperatures: (a) Young's modulus; (b) CTE。

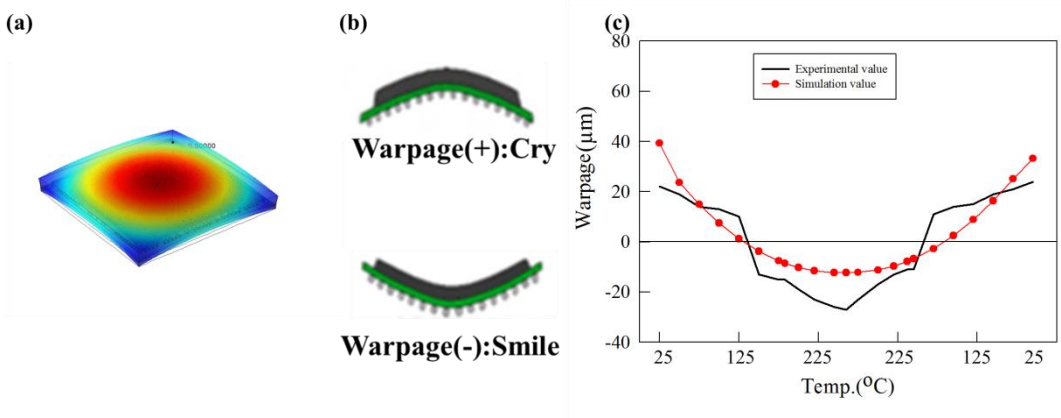


Fig. 2: (a) single unit simulation model ; (b)warpage cry(+) and smile(-) ; (c) experimental value and simulation value of shadow moire.

Contribution

This study successfully simulated the single unit warpage for the shadow moire measurement in Flip-Chip process. Fig. 2 illustrates single unit warpage of simulation model and results. This study found that the simulation value match the experimental value very well, which the trend of deformation is consistent. According to the aforementioned, this simulation method can be used to estimate the single unit warpage. Furthermore, it can help to improve process yield and keep the cost down on the production line.

Keywords: CTE, Single unit warpage, Flip-Chip, Shadow moire

References

[1] S. J. Oon, K. S. Tan, T. Y. Tou, S. S. Yap, C. S. Lau, and Y. T. Chin, "Warpage Studies of Printed Circuit Boards with Shadow Moiré and Simulations," in 2018

IEEE 38th International Electronics Manufacturing Technology Conference (IEMT), 2018, pp. 1-5

Efficient and accurate two-scale FE-FFT-based prediction of polycrystalline material behavior at finite strains

Christian Gierden[1], Julian Kochmann[1,2], Johanna Waimann[1], Bob Svendsen[1,3], Stefanie Reese[1]

[1]RWTH Aachen University, [2]MTU Aero Engines AG, [3]Max-Planck-Institut für Eisenforschung GmbH

christian.gierden@rwth-aachen.de, julian.kochmann@rwth-aachen.de, johanna.waimann@rwth-aachen.de, b.svendsen@mpie.de, stefanie.reese@rwth-aachen.de

In order to capture a complex heterogeneous material behavior in structural finite element simulations, the application of a two-scale simulation approach is required to account for individual microstructural effects. In this context, former studies [1] already show that the recently developed FE-FFT method (e.g. [2]) seems to be more efficient than the common FE² method (e.g. [3]). However, the computational effort for a two-scale simulation is still extremely high. In order to reduce this effort, more efficient methods, e.g. FFT-solvers in combination with model order reduction techniques [4], are necessary. We present an efficient FE-FFT-based simulation approach for the prediction of the local and overall mechanical behavior of polycrystalline materials, which is introduced by Kochmann et al. [5], and extend this simulation approach for finite strains and for more general microstructures.

The proposed solution scheme is decomposed into three steps: (i) pre-processing, (ii) processing and (iii) post-processing. In the pre-processing step a convergence analysis in terms of the macroscopic stress is performed by considering different discretizations and thus a different number of grid points in each direction (see Figure 1). The result of this pre-processing step is a minimal number of grid points that must be considered to obtain a solution with an error which is

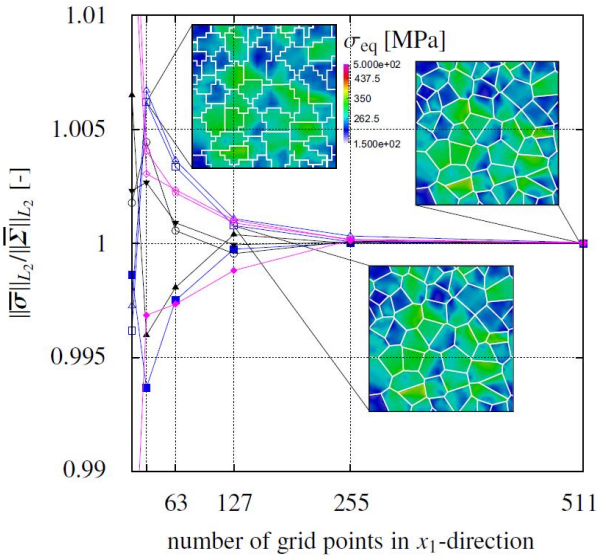


Figure 1. Error in the macroscopic stresses of different discretized microstructures for different load cases [5].

(compared to the converged solution) smaller than a prescribed tolerance. Secondly, in the processing step, the two-scale full-field simulation is performed using the coarse discretization of the minimal number of grid points. Within this simulation, the macroscopic strain tensor is stored at every macroscopic integration point of particular interest. Finally, in the post-processing step, highly resolved microstructure data are generated by applying the stored macroscopic strain tensor to a fine discretized microstructure.

In order to demonstrate the versatile use of the proposed approach, polycrystalline materials with different textures and different intrinsic anisotropy are considered. On this basis and as a first representative simulation, the micromechanical fields and the related overall material behavior of body-centered cubic (bcc) polycrystals are predicted for simple macroscopic boundary value problems.

References

[1] Prakash, A., Lebensohn, R.A., 2009. Simulation of mircomechanical behavior of polycrystals: finite elements versus fast Fourier transfomrs. Modelling and Simulation in Material Science and Engineering 17, 16pp.

[2] Kochmann, J., Wulfinghoff, S., Reese, S., Mianroodi, J.R., Svendsen, B., 2016. Two-scale FE-FFT- and phase-field-based computational modeling of bulk microscructural evolution and macroscopic material behavior. Computer Methods in Applied Mechanics and Engineering 305, 89-110.

[3] Smit, R.J.M., Brekelmans, W.A.M., Meijer, H.E.H., 1996. Prediction of the mechanical behaviour of nonlinear heterogeneous systems by multi-level finite element modeling. Computer Methods in Applied Mechanics and Engineering 155, 181-192.

[4] Kochmann, J., Manjunatha, K., Gierden, C., Wulfinghoff, S., Svendsen, B., Reese, S., 2018. A simple and flexible model order reduction method for FFT-based homogenization problems using a sparse sampling technique. Computer Methods in Applied Mechanics and Engineering 347, 622-638.

[5] Kochmann, J., Wulfinghoff, S., Ehle, L., Mayer, J., Svendsen, B. Reese, S., 2017. Efficient and accurate two-scale FE-FFT-based prediction of the effective materialbehaviour of elasto-viscoplastic polycrystals. Computational Mechanics 61, 751-764.

Diffusion-Kinetic Monte Carlo Methods for Neutral Transport in Plasma Edge Simulations of Nuclear Fusion Reactors

Bert Mortier[1], Martine Baelmans[2], Giovanni Samaey[1]

[1]KU Leuven, Department of Computer Science,
[2]KU Leuven, Department of Mechanical Engineering

bert.mortier@kuleuven.be

Economically viable nuclear fusion would provide a sustainable energy source for our planet, with nearly limitless resources and virtually no radioactive waste. A lot of progress is yet to be made, with ITER [1] and DEMO [2] reactors as the next important steps. The design of these reactors requires simulation of the plasma and its interaction with the solid components. Of these solid plasma-facing components, the divertor target receives the highest energy flux from the plasma. In a so-called detached regime, a relatively dense neutral mass cushion in front of the divertor limits the energy flux carried by ions towards the divertor target. To estimate these fluxes and the effectiveness of the cooling, simulations of the plasma edge are particularly important.

In a detached regime, the neutrals in the plasma edge traverse regions of high collisionality before being absorbed by the plasma in neighbouring regions of medium and low collisionality. The neutrals are modeled by a kinetic equation, discretized by a stochastic particle (Monte Carlo) method. In a high collisional regime, a kinetic simulation is expensive, since the Monte Carlo method requires resolving each individual collision. In that regime, however, a limiting fluid equation exists, which only considers mass, momentum and energy as a function of space and time. Such a fluid model is cheaper to simulate, but results in large errors when the collisionality is low.

We propose a modified simulation of the kinetic equation that uses a fixed time step Δt in which the individual collisions are aggregated into a diffusion step, resulting in a bounded simulation cost per time step. This aggregation is performed by taking a Brownian motion (diffusion) step of which the mean and variance correspond to the mean and variance of a kinetic simulation during the same time interval. Furthermore, potential large deviations by the first flight are resolved by taking an initial kinetic step, resulting in $O\left(\Delta t^{3/2}\right)$, $\Delta t \to 0$ convergence to the kinetic simulation. By including an additional kinetic step, an $O(\Delta t^3)$, $\Delta t \to 0$ convergence to the kinetic simulation is attained, for a small increase in simulation cost.

[1] Kukushkin, A. S., et al. "Finalizing the ITER divertor design: The key role of SOLPS modeling." *Fusion engineering and design*86.12 (2011): 2865-2873.

[2] Subba, F., et al. "Preliminary analysis of the efficiency of non-standard divertor configurations in DEMO." *Nuclear Materials and Energy* 12 (2017): 967-972.

Development of a simple ergodic stochastic representative volume element for heterogeneous materials with random geometry of microstructure

Dmytro Pivovarov [1], Kai Willner [1], Paul Steinmann [1]

[1] Chair of Applied Mechanics, Friedrich-Alexander University Erlangen-Nürnberg

dmytro.pivovarov@fau.de

Due to high computational costs associated with stochastic computational homogenization, the highly complex random material microstructures are replaced often by some simplified, parametric, ergodic and sometimes periodic models. This replacement is often criticized in the literature due to unclear error resulting from periodicity and ergodicity assumptions. In this work we propose an approach to design this kind of simplified models for heterogeneous materials with randomly distributed inclusions with random radii, which demonstrates a good agreement with full-scale non-ergodic simulations. Proposed model design is based on some assumptions: dominating role of volume fraction in determination of homogenized quantities, ergodicity assumption, and priority of the interparticle distances over other microstructural characteristics. Accuracy of the presented simplified model is validated through a numerical example.

Multi-uncertainty analysis of the indentation process of key engineering materials

T.L. Amaral, T. Doca[1]

[1]University of Brasilia, doca@unb.br

Indentation tests are often used to obtain surface properties, such as hardness [1], and can also be employed for the mechanical characterization of a material [2,3]. These tests require equipment with multiple known sources of uncertainty. For instance, the input of axial force is bound to the error of a loading cell while the displacement sensor is affected by disturbances in the servo-hydraulic system. These uncertainties contributes to the overall dispersion of the results, in this case, the depth and width of an indentation mark.

An assessment of the influence of these uncertainties is presented. The compression tests are performed using a MTS 809 and sample holder device. A sphere-to-flat contact configuration is chosen. Tests are carried-out in the both the elastic regime and after the onset of inelastic strains. The indentation marks are measured with a confocal laser microscope. Four different materials are analysed: CA6NM stainless steel, R3 grade offshore steel, Polycarbonate (PC) and a blend of PC and Acrylonitrile Butadiene Styrene (ABS).

The four sources of uncertainty studied are: i) variation of the Elastic modulus; ii) error of the loading cell; iii) error of the displacement sensor; iv) error of the measured dimensions of the indentation mark. The experimental data is compared to numerical predictions [4] and analytical results [5-6] to evaluate the correlation between these different types of analyses.

References

[1] H Chandler. Hardness testing. Cleveland: ASM International; 1999.

[2] MB Toloczko, ML Hamilton, GE Lucas. Ductility correlations between shear punch and uniaxial tensile test data. J Nucl Mater, 283 (2000)

[3] RK Guduru, KA Darling, R Kishore, RO Scattergood, CC Koch, KL Murty Evaluation of mechanical properties using shear-punch testing. Mater Sci Eng A, 395 (1–2) (2005)

[4] T Doca, FM Andrade Pires, JMA César de Sá. A frictional mortar contact approach for the analysis of large inelastic deformation problems. Int J Solids Struct; 51:1697–715 (2014).

[5] R Hill. The mathematical theory of plasticity.Oxford:Oxford University Press Inc.; 1950.

[6] KL Johnson, Contact mechanics, Cambridge University Press, 1987.

Adjoint Based Optimisation of an Internal Cooling Channel U-Bend

Jens-Dominik Müller [1], Oluadamilare Imam-lawal [1], Tom Verstraete [2]

[1]Queen Mary, University of London, Von Karman Institute for Fluid Dynamics

ghanem@usc.edu

Conjugate Heat Transfer (CHT) is a multidisciplinary problem which occurs when heat is transferred between a fluid and a solid. Numerical optimisation of CHT problems has mainly used gradient-free methods which is limited to a small number of design variables [1]. Alternatively, gradient-based optimisation can handle large design spaces, and are very economical if gradients are computed with the adjoint method. While the use of adjoint methods is common for single disciplines, it is a recent field of interest in CHT [2].

CHT problems may be solved in a partitioned manner where separate solvers are used for both domains and the exchange of boundary conditions between solvers is required [3]. The use of partitioned coupling and adjoint methods for CHT optimisation presents an interesting challenge as it requires the differentiation of the numerical solvers and their coupling. The exchange of boundary conditions and adjoint gradients between the solvers is dependent on the type of coupling method used. In this work, we make use of Automatic Differentiation (AD) to obtain adjoint gradients. The paper will present the application of AD to the solvers, as well as and the differentiation of the coupling boundary conditions, resulting in a consistent exchange of gradients between solvers.

We consider an optimisation problem in which the goal is to reduce the pressure loss in a U-Bend cooling channel [3,4]. This is achieved by performing a gradient-based optimisation to change the shape of the cooling channel. The results are obtained using the open-source structural solver CalculiX and the in-house flow solver STAMPS. The results show how the discrete adjoint method obtained using AD can be effectively combined with partitioned CHT methods to solve optimisation problems.

References

[1] Ping He and C.A. Mader and J.R.R Martins and K.J. Maki, “Aerothermal optimization of internal cooling passages using a discrete adjoint method." *AIAA*, (2018).

[2] K.T. Gkaragkounis and E.M. Papoustis-Kiachagias and K.C. Giannakoglou , “The continuous adjoint method for shape optimization in Conjugate Heat Transfer problems with turbulent incompressible flows." *Applied thermal Engineering*, 140 (2018), pp (351-362).

[3] T. Verstraete, F. Coletti, J. Bulle, T. V. der Wielen, and T. Arts. Optimization of a U-Bend for Minimal Pressure Loss in Internal Cooling Channels Part I: Numerical Method. ASME Journal of engineering for Gas Turbines and Power, 135:pp 051015, 2013.

[4] F. Coletti, T. Verstraete, J. Bulle, T. V. der Wielen, N. van den Berge, and T. Arts. Optimization of a U-Bend for Minimal Pressure Loss in Internal Cooling Channels – Part II: Experimental validation. ASME Journal of engineering for Gas Turbines and Power, 135:pp 051016, 2013.

System time-variant reliability-based structural design optimization of deteriorated truss bridges

Younes AOUES[1], Didier LEMOSSE[1], Eduardo SOUZA DE CURSI[1]

[1]Normandie Univ, INSA Rouen Normandie, LMN, France.

Younes.aoues@insa-rouen.fr

The CLASSE2 project focuses on the performance conditions of supply chains and the reliability of the logistic corridors of the Normandy region. The fluidity of logistics corridors depends mainly on the reliability of infrastructures transportations. Highway bridges are considered the most critical and vital links in any transportation network, where a full or partial failure of these infrastructures leads to decrease the operational efficiency of the network and can provoke serious economic impacts. These infrastructures undergo various degradation (decay, aging, corrosion, fatigue) due to the weather conditions, natural disaster, the increase in traffic of the last decades.

In the current economic context, design optimization is usually applied to cost reduction and to improve structural performances. The optimal design is generally searched by minimizing the structural cost and checking performance criteria and the design requirements. The reliability-based design optimization (RBDO) approach aims to find the best compromise between the structural cost and safety assurance [1]. The RBDO approach is based on considering uncertainties related to geometry, material properties and approximation models that affect the structural system.

Bridges are subjected to various deterioration processes that reduce their structural performance significantly during their long-term performance (e.g., decay, aging, corrosion, fatigue, etc.). The structural deterioration is a major problem for many companies and countries, where important costs are involved to maintain, repair or to replace the deteriorated structures. Therefore, when structures are subjected to degradation during their lifetime, the RBDO approach should consider the time-dependency of load and environmental fluctuations. This time-dependency can be considered by using a time-variant reliability analysis where load and environmental variables are modelled by stochastic processes [2]. However, the failure of the truss structures is devoted to several failure modes (i.e. several limit state functions) [3]. Thus,

the time-variant RBDO approach may consider the overall system reliability (i.e. a combination of several limit states) instead of the single component reliability (i.e. single limit state function).

This study presents a new methodology for the system time-variant reliability-based design optimization, where the system time variant reliability is estimated on the basis of the time-variant limit state functions. In order to alleviate the computational time of the RBDO procedure [4], the system time variant reliability analysis is decoupled from the optimization procedure. In other words, the proposed approach is based on transforming the system time variant RBDO problem into a sequence of equivalent deterministic design optimization sub-problems. This transformation is defined by the mean of optimal safety factors, linking the reliability requirement to the equivalent deterministic optimization. At the end of each sub-problem optimization, the reliability constraint is verified by performing a system time-variant reliability analysis. The safety factors corresponding to the target reliability level at the desired lifetime are calibrated by an inverse probabilistic approach. Finally, these safety factors are provided to the following sub-problem of the equivalent deterministic optimization and so on, until convergence. This approach is applied to find the optimal design of truss bridges subjected to degradation. The overall results indicate that the system performance of the optimized truss ensures the target reliability level during the whole structural lifetime.

REFERENCES

[1] Frangopol, D.M., Moses, F. 1994. Reliability-based structural optimization. Adeli H, editor. Advances in design optimization. London:Chapman Hall.

[2] Kuschel, N., Rackwitz, R. 2000. Optimal design under time- variant reliability constraints. Structural Safety 22(2): 113-27.

[3] Aoues, Y., Chateauneuf, A., Lemosse, D., El-Hami, A. 2013. Optimal design under uncertainty of reinforced concrete sturcutres using system reliability appraoch, International Journal for Uncertainty Quantification 3(6): 487–498.

[4] Aoues, Y., Chateauneuf, A., Benchmark study of numerical methods for reliability-based design optimization, Structural & Multidisciplinary optimization 2010;41(2):277–294.

Examining the Mutation Effect of SLC26A4 STAS Domain By Observing the Communication Between Secondary Structures

Hyun Joon Chang [1], Jae In Kim[2], Sungsoo Na[1*]

[1]University of Southern California

[2]Hyundai Steel Company

[*]nass@korea.ac.kr

The mutation of STAS domain within Pendrin (SLC26A4), a protein associated with the auditory system, causes typical auditory disorders such as Pendred syndrome (PDS) and DFNB4. In this study, we generated six mutated STAS domain models related to PDS, DFNB4, and PDS/DFNB4 as well as the wildtype model, and performed Molecular dynamics simulations to find the difference in equilibration conformation and fluctuation information. We used network analysis on a residue-residue scale to calculate betweenness centrality and edge betweenness, and further scaled up to secondary structures to reveal the communication map within the STAS domain. Our results showed that the communication signals generated by the mutated models are less clear than those of WT model.

Presenting Author, Second Author, Corresponding Author

New Vortex Identification Methods - Omega, Liutex/Rortex, Omega-Liutex

Chaoqun Liu [1]

[1]University of Texas at Arlington, Arlington, Texas, USA

cliu@uta.edu

Vortex is intuitively recognized as the rotational/swirling motion of the fluids, but a universally accepted definition of vortex is still not available. In thousands of research papers and almost all textbooks, vorticity tube/filament is regarded equivalent to vortex and the magnitude of vorticity is deemed the strength of vortex, which is a misunderstanding of the vortex nature since Helmholtz (1858). During the last three decades, a lot of vortex identification methods, including Q-, Δ-, λ_2-, λ_{ci}- criteria, have been developed. Most of these criteria are based on Cauchy-Stokes decomposition and/or eigenvalues of the velocity gradient tensor. Starting from 2014, the Vortex and Turbulence Research Team at University of Texas at Arlington (UTA Team) focus on the development of a new generation of vortex identification methods. A new Omega vortex identification method, which defined the vortex as a connected region where vorticity overtook deformation, was published in 2016 [Liu et al, New omega vortex identification method, Science China: Physics, Mechanics & Astronomy, 2016, 59(8): 684711]. The Omega method has several advantages: (1) easy to perform, (2) clear on physical meaning, (3) non-dimensional and normalized from 0 to 1, (4) robust to threshold change, (5) able to capture both strong and weak vortices simultaneously. In 2017 and 2018, a Liutex (previously called Rortex) vector was proposed by UTA Team to represent the local rigid rotational part of fluid motion, which is a mathematical definition with its direction as the local rotational axis and its magnitude as the rigid rotation strength [Liu et al, Rortex—A new vortex vector definition and vorticity tensor and vector decompositions Physics of Fluids 30, 035103 (2018); doi: 10.1063/1.5023001]. Liutex/Rortex is

a new physical quantity with scalar, vector and tensor forms exactly representing the local rigid rotation of fluids. Meanwhile, a decomposition of vorticity to a rotational part namely Liutex/Rortex and an anti-symmetric shear part (RS decomposition) was introduced in 2018 and a velocity gradient tensor decomposition to a rotation part (R) and a non-rotation part (NR) which could be further decomposed as pure shearing (PS) and stretching and compression (SC) was given in 2019 [Gao and Liu, Rortex based velocity gradient tensor decomposition, Physics of Fluids, Phys. Fluids **31**, 011704 (2019); https://doi.org/10.1063/1.5084739] as a counterpart of Cauchy-Stokes decomposition. Later in early 2019, a Liutex/Rortex based Omega method called Omega-Liutex [Dong, Gao and Liu, New normalized Rortex/vortex identification method, Physics of Fluids 31, 011701 (2019); doi: 10.1063/1.5066016] was developed, which combines the advantages of both Liutex and Omega methods. These breakthroughs in the development of vortex science by UTA Team are classified as a new generation of generation of vortex identification methods. The critical problems for vortex identification concern with the vortex core location, vortex core size, vortex boundary and size, absolute vortex strength, relative vortex strength, mixture of strong and weak vortices, vortex rotation axes, etc. Only the new third generation of vortex identification methods can answer these questions while all the other vortex identification methods fail to answer all questions except for part of the first one (approximate vortex boundary when the threshold is extremely small). The talk will introduce the new vortex identification methods including Omega, Liutex/Rortex, Omega-Liutex. **A numeber of computational examples by using the new vortex identification methods for flow transition and turbulence will be reported.**

Presenting Author, Chaoqun Liu, cliu@uta.edu

Multi-scale and Multi-physics challenges for Future Aircraft: A Hierarchical Approach

Paul G. Tucker [1]

[1]University of Cambridge

Pgt23@cam.ac.uk

The various multi-scale and multi-physics modelling needs of future aircraft are discussed. In a hierarchical fashion both the handling of the inevitable turbulent flow and geometry are considered. The latter is necessary to help more economically deal with the increasingly coupled nature of many aerodynamic problems and also the drive towards considering ever increasing levels of geometrical complexity. The proposed unified framework could be exploited all the way though initial fast preliminary design to final numerical test involving various bespoke combinations of hierarchical components.

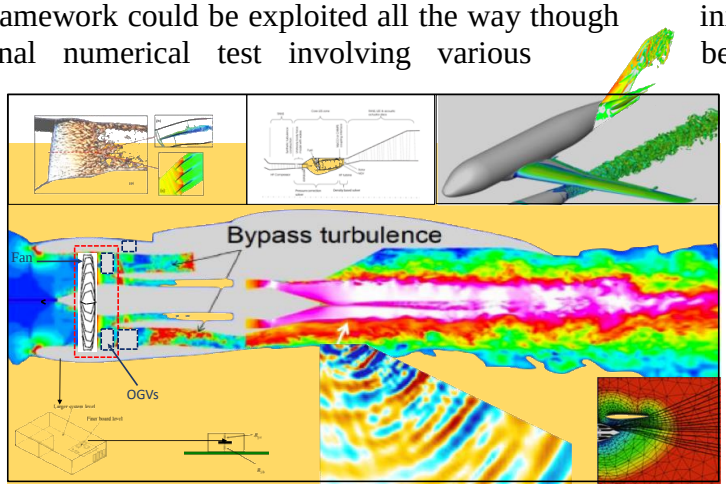


Figure 1. Multi-scale elements of modern aircraft and their engines.

The aircraft engine is inherently a multi physics system. Fuel is burned. This generates aerodynamic forces which in turn drives the turbine and ultimately creates aerodynamic thrust. The combustion system in a modern aircraft engine is also inherently multiscale but this time as a sub-system. Its design intent is to generate large scale turbulence which itself generates subsequently smaller turbulent scales. Fuel is mixed into these scales the fuel is broken down into droplets. The combustion process, from the ignited droplets, results in a flame front. This fine front has wrinkling. The smaller more complex this wrinkling the more efficient the combustion process. Efficiency of the combustion process and the aerodynamics together is of clearly of vital importance with respect to global warming. By 2025 there will be around 1 billion tonnes of annual CO_2 emissions from aircraft alone. Naturally the aircraft engine is tremendously powerful and this results in the generation of substantial aerodynamic noise. The reduction of this noise is the second major aerospace priority in the US and Europe. The aeroelastic response of the components in the aircraft system at a wide range of scales is also an area of considerable importance. Hence, the system is clearly multiphysics. The engine itself is intrinsically a multi scale system. For example, the diameter of the engine is around 2 m and this roughly corresponds to the diameter of the fan at the front of the engine. Figure 1 shows selected multi-scale elements of modern aircraft and their engines. Most of the thrust comes from the fan which for the purposes here can be considered as *e*ffectively a propeller. After the fan there are blades that compress the air *leading to the combustor*. The energy liberated by this drives the turbine

which in turn drives the fan, any residual energy is used as thrust coming out of the back of the engine in the form of a jet - called the propulsive jet.

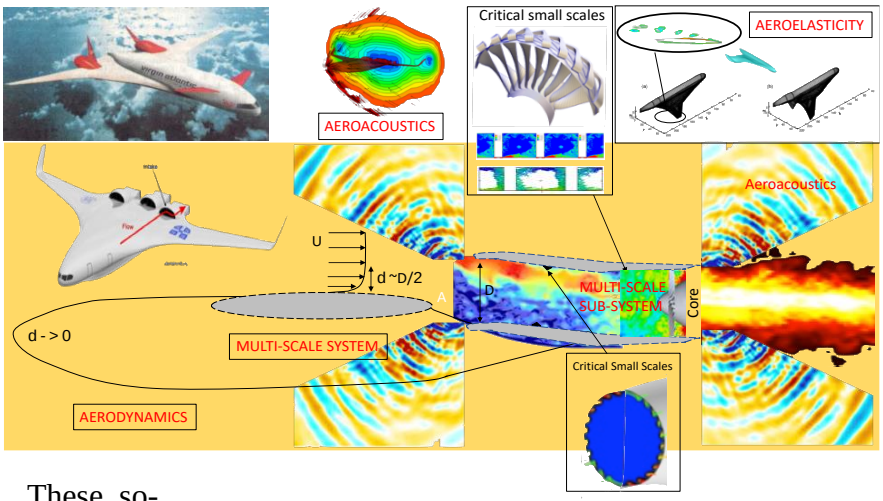


Figure 2 Multi-scale elements of future blended wing-body aircraft.

Since the fan also compresses the air, like the compressor, there is a risk of the air flowing backwards. This is often mitigated by using fine intricate structures embedded in the shroud geometry above the tips of these components. These so-called casing treatments are shown in figure 2 (top row, 3rd element along from the left). The casing treatments can range from geometries involving simple grooves, to far more complex multi-scale configurations. The disparity in scale between the fan and these grooves is many orders of magnitude. Figure 3 shows the core of an engine. Consisting of the compressor stages, combustor and subsequesnt turbine. The turbine is also, in itself, is a problematicaly multi-scale system. The largest disparity in geometrical scale is that of the blade chord (or span) to the fine holes that shield the surface from hot gasses from the combustion. This ratio is around 1000. Suface roughness from wear is important to the turbine blade increasing surface skin friction by 80%. The inside of the turbine balde has complex multiscale cooling eleements. The balde extremeities also have coplex seals. All these elements are shown in Figure 3.

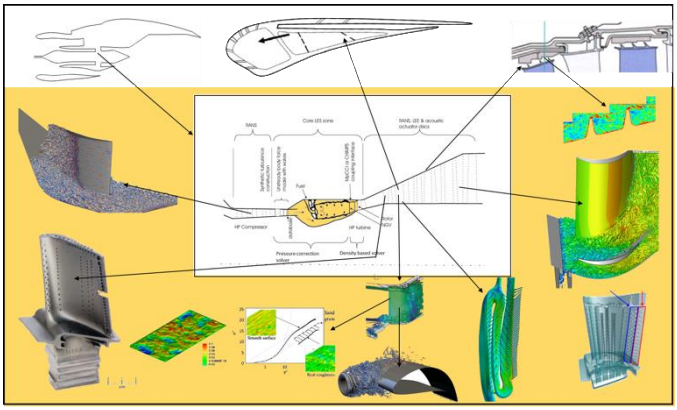


Figure 3. Multi-scale elements of turbine.

Here it is proposed to deal with the above noted multi-scale and physics challenges using hierachical modelling for both turbulence and geometry. For futurue aircraft this is especially important since the airframe and engine are becoming ever more closely integrated. This can be seen to a degree in the next generation as shown in Figure 1 and far more fully in the future – see Figure 2.

Probabilistic Design Optimization for CO2 Storage with Leakage Risk Control

Ben Mansour Dia[1] and Bilal Saad[2]

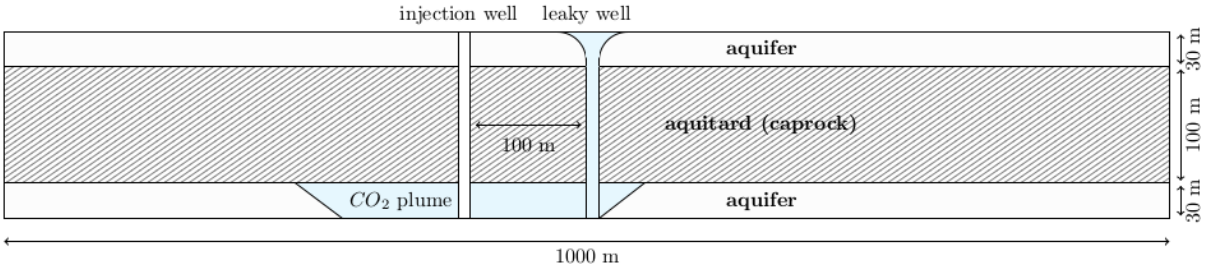
[1]CPG, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

[2]Baker Hughes Research Center, Dhahran Techno Valley, Dhahran, Saudi Arabia

diabenmansour@gmail.com

The physical process of CO2 injection in geologic reservoirs, including solubility trapping, is a non-isothermal two-phase two-component flow in porous media, which is governed by a system of coupled nonlinear partial differential equations [2]. In this model, the water-rich phase (brine) and the carbon dioxide-rich phase (CO2) consist of two components (water and CO2 component), as the solubility of the components in the phases has to be taken into account. Local equilibrium phase exchange of the components in the phases is assumed to hold. To close the system, the fluid properties of CO2 are calculated as functions of pressure and temperature.

For simulations purpose, a reservoir composed of two aquifers separated by an aquitard is considered. The leaky well is modeled as a porous medium with higher permeability compared to the rest of the formation. We count the effect of uncertainties in reservoir porosity, reservoir absolute permeability, and permeability of the leakage well, on the model response. Also, we consider spatial heterogeneity only through the different layers according to different geological media, and we count the changes in fluid properties of CO2, and that the CO2 and brine fluid properties (e.g., density and viscosity) depend on the aquifer conditions, the temperature, the CO2 pressure, the brine salinity, and the mass fraction of CO2 in brine.



In the talk, we present scenario where CO2 is injected to be stored in the lower aquifer and the injected CO2 spreads within the aquifer and once it reaches the leaky

well, it connects the two aquifers and rises to the shallower aquifer. The following sketch summarizes the model geometry and illustrates a 2D section of the 3D domain. We address an optimal experimental design problem under uncertainties, [1,3], with the main objective of searching the optimal injection rate of CO2 for the learning of the leakage rate in order to consistently maintain the harmful leakage risk.

References

[1] C. Thimmisetty, P. Tsilifis, R. Ghanem, Homogeneous chaos basis adaptation for design optimization under uncertainty: Application to the oil well placement problem. *Artificial Intelligence for Engineering Design, Analysis and Manufacturing (2017), 31, 265–276.*

[2] B. M. Saad, A. Alexanderian, S. Prudhomme, O. M. Knio, Probabilistic modeling and global sensitivity analysis for CO 2 storage in geological formations: a spectral approach. *Applied Mathematical Modelling 53 (2018) 584–601*

[3] J. Beck, B. M. Dia, L. F. R. Espath, Q. Long, R. Tempone, Fast Bayesian experimental design: Laplace-based importance sampling for the expected information gain. *Computer Methods in Applied Mechanics and Engineering 334 (2018) 523–553.*

Development of Multiscale Multi-physics Based Modelling and Simulations with the Application to Precision Machining of Aerofoil Structures

Kai Cheng[1], Yizhi Shao[1] and Rodrigo Bodenhorst[1]

[1]Brunel University London

Kai.cheng@brunel.ac.uk, Yizhi.shao@brunel.ac.uk

Multiscale multi-physics based modelling and simulations are getting more and more interest by the industry and research community particularly in the context of increasing demands for high precision manufacturing and complex production environment. With the development of multiscale multi-physics based modelling and simulation, it will enable effective and efficient optimisation of the manufacturing process and further improvement of the production in terms of quality, costs, shortest delivery and overall competitiveness. In this paper, some basic models and analysis using multiscale multi-physics modelling are presented and discussed. Furthermore, the possibility of adopting the multiscale multi-physics modelling and simulation to the virtual machining system is evaluated, and further supported with an industrial study case study on Abrasive Flow Machining (AFM) of integrally bladed rotors (IBR) using the modelling and simulation techniques above.

An Investigation of Stepwise Crack Tip Advancement

Yanan Sun[1], Bin Chen[2], Michael G Edwards[1], and Chenfeng Li[1]

[1]Swansea University

[2]Imperial College London

966781@.Swansea.ac.uk

This research focuses on stepwise crack tip advancement associated with hydraulically induced fractures, which are observed both in the field and in experiments and reported in the numerical fracture modelling literature.

A numerical model of hydraulic fracture in porous media is established. The finite element method is employed to solve the fully coupled equation system, which includes rock deformation, fluid flow in both the fracture and rock matrix and fracture propagation. To reproduce the stepwise phenomenon, a special time stepping scheme is used, which allows for multiple incremental fracture advancement within a time step according to a cohesive stress constraint. With the model, the contributing factors to the stepwise phenomenon are studied, and a numerical sensitivity analysis of this phenomenon is presented.

The contributing factors are summarized, including Young's modulus, Poisson's ratio, Biot's coefficient, Biot's modulus, rock porosity and permeability, viscosity, injection rate and fracture toughness. Among all the factors, Young's modulus, permeability, injection flow rate, fluid viscosity and fracture toughness are found to be predominant. A further key contributing factor is that the velocity of solid deformation is much faster than fluid deformation. This study helps to understand the influence of different factors to the stepwise phenomenon and provides possible explanations behind this phenomenon.

Dynamic Analysis of a Multi-Contact Problem

Using Simplified Models to Study of the Influence of Clearances on Contact Forces

Thomas Catterou [1], Victor Blanc[1], Guillaume Ricciardi[2],

Stéphane Bourgeois[3], Bruno Cochelin[3]

[1]CEA Cadarache, DEN/DEC/SESC/LECIM, F-13108 Saint Paul Lez Durance, France

[2]CEA Cadarache, DEN/DTN/STCP/LTHC, F-13108 Saint Paul Lez Durance, France

[3]Aix Marseille Univ., CNRS, Centrale Marseille, LMA, Marseille, France

victor.blanc@cea.fr

The purpose of this paper is to show the efficiency of a simplified multi-body system in order to analyze dynamic response of a multi-component system with clearances. Initially, a 2D multi-contact model based on beam finite element model and a modal basis reduction has been developed in order to compute the global response of a nuclear fuel subassembly submitted to a shock. The assessment of contact forces that occurs between sub-components must be conservative, but, as already observed in the literature, results show that the evolution of the contact forces with initial joint clearances is clearly non-linear and presents a maximum for small gaps values, what is counter-intuitive.

In order to reduce computational costs and to analyze the effects of initial joint clearances by a parametric study, a simplified spring-mass system is presented in this paper. Characteristics of the simplified model are chosen using an analysis of the spectral response of the finite element model. The simplified model is dimensionless using first modes of vibration of the components.

First, we observe that physical phenomena, which causes the chaotic response described by the finite element model are very well reproduced by the simplified multi-body system. In addition, as observed with the finite element model, contact forces present a maximum for small values of the initial gaps. Characteristic times of compression waves and of local contacts oscillation are very close to the detailed model.

Secondly, phenomenology of the forces transfer between masses is analyzed, and related to the initial gaps values. The displacements are also analyzed, and their evolution

allow us to understand phenomenon that causes the increase of the contact forces for small gaps values. This result shows the interest of such simplified model in order to explain complex physical phenomena occurring inside these structures.

A phase-field damage model with micro inertial effect for dynamic failure of quasi-brittle materials

Lu Hai[1], Jie Li [2]

[1]Tongji University

tjhailu@tongji.edu.cn

[2]Tongji University

lijie@tongji.edu.cn

The prediction of the structural response and failure under dynamic loadings such as blast and impact is of particular importance to the design of concrete structures. Various theoretical models, based on the plasticity theory, fracture and damage mechanics, etc., have been developed to characterize the dynamic mechanical behavior of concrete. Compared to quasi-static loading, quasi-brittle materials subjected to high-rate loading exhibit the rate-dependency due to the inertial effects at multiple scale levels. The resistance, failure mode and crack pattern are sensitive to the strain rate, which is the main challenge when developing a continuous model for dynamic failure.

Recently the phase-field method for damage and failure in solids has attracted extensive theoretical and computational investigations. With extension to quasi-brittle failure, the researches indicate that the phase-field model can predict the global responses of concrete structures under static loads accurately, e.g. load-displacement curve and crack path. However, the phase-field model for dynamic failure of concrete still remain an open and challenging issue. The rate-dependency of materials is not considered in existing models.

To overcome the above problem, we introduce the micro inertial mass to consider the physical mechanisms of strain-rate sensitivity in this contribution. Based on Hamilton principle, a novel phase-field damage model with microscale inertial effect is proposed. The model performance is tested with two sets of numerical examples including compact tension tests and spall tests of concrete at high strain rate. Good agreement is achieved with numerical results and experimental results; and particularly the rate-dependency of concrete subjected to high-rate loading can be investigated with this model.

Two-scale phase field modeling of damge and fracture for disordered media

Ye Feng [1] and Jie Li [2]

[1] Tongji University, Shanghai, China

1710181@tongji.edu.cn

[2] Tongji University, Shanghai, China

lijie@tongji.edu.cn

As a continuum field description, phase field method provides possibility to describe the complex evolution of crack fronts without any extra computational efforts to track crack path. In phase field modelling, an order parameter is used to describe the local damage state of material. The order parameter is taken zero in intact phase and some positive value in "broken" phase. The key idea is to regard damage and fracture evolution as a process that spontaneously reduces the total free energy, which can be written as a functional of displacement field and order parameter field (or phase field). This idea can be conveniently implemented in finite element method after using variation principle.

In principle, phase field method is valid at any scale as long as the "infinitesimal" volume in the model can still be regarded as macroscopic element that contains huge number of particles. However, a very fine mesh is required to capture the diffusion of crack surface, because the thickness of the real crack surface is only a few molecules radius width. In practical, the thickness of crack is controlled by a numerical parameter and the surface energy density, which related to the total free energy minus elastic energy, is controlled as constant. A variety of phase field models have been proposed for ideal brittle homogenous media, where the surface energy density (or fracture strength) is a constant field. However, many practical materials, such as concrete, bone and ceramics, are heterogeneous and the fracture strength should be treated as a random field. The macroscopic mechanical behaviors are quite different between homogenous material and random media.

This talk will describe recent efforts at developing a two-scale phase field method of damage and fracture for discorded media, where the fracture strength is assumed as a random field with a very small correlation length. A discrete lattice model is introduced as a bottom model to derive the probability information of "damage potential" which is part of the total effective free energy. Then a macroscopic phase field model is developed

based on the information given by bottom lattice model. Numerical examples are given to show the property of the proposed method. The results show that the proposed method can reproduce phenomenon such as crack surface roughening and the random behavior in force-displacement curve.

The Refined Algrithm of Generalized Probability Density Evolution Equation Based on Reproducing Kernel Particle Method

Dan Wang [1,2] and Jie Li [1,3]

[1]Tongji University

[2]wangdan1995@tongji.edu.cn

[3]lijie@tongji.edu.cn

The generalized probability density evolution equation (GDEE) is a partial differential equation governing the evolution of the joint probability density function (PDF) of the response of interest and the source random variables, which holds for both linear and nonlinear stochastic dynamic systems. It's worth mentioning that the randomness involved in the initial conditions, excitations and structural properties can be taken into account simultaneously in the GDEE. Besides, the dimension of the GDEE is only dependent on the dimension of the quantity of interest, and nothing to do with the dimension of the stochastic dynamic system itself. The traditional numerical solving process of the GDEE, referred to as the probability density evolution method (PDEM), has been systematically developed, which has been applied to many areas, e.g., structural system reliability evaluation and stochastic optimal control, etc.

The key factor limiting the accuracy and efficiency of the tradition PDEM is the number of representative points required. On one hand, to alleviate the problem of mesh sensitivity, a large number of representative points should be selected. On the other hand, the step of deterministic analysis is computationally expensive to implement, especially for a complex structure involving high dimensionality and strong nonlinearity.

This talk will describe recent efforts at developing a numerical method for overcoming the above limitations, named the refined algorithm based on reproducing kernel particle method (RKPM), in which a surrogate model method and the PDEM are combined. By this method, the instantaneous probability distributions of the quantities of interest can be obtained. The problem of mesh sensitivity is settled well, and the accuracy is relatively high. Besides, the computational efforts are considerably reduced. The accuracy and efficiency of this method is verified by some numerical examples.

Data-Drive Approaches in Predicting Premixed Reactive Flow

Mohsen Ayoobi [1] and Ali Takbiri-Borujeni [2]

[1]Wayne State University and [2]West Virginia University

mohsen.ayoobi@wayne.edu, ali.takbiriborujeni@mail.wvu.edu

Complex interplays of different physical phenomena including ignition, chemical kinetics, turbulence, etc. make the computational simulation of combustion-related applications challenging in practical cases and therefore, researchers have to overlook some details and rely on simplistic models. For example, in order to decrease the computational expenses (memory and time), one may have to disregard the detailed chemistry, or filter the flame interactions with the flow and eddy structures at smaller scales. Such assumption limit the combustion-related applications that can be simulated with confidence in their accuracy. This study aims at employing Artificial Intelligence (AI) and more specifically Machine Learning (ML) techniques to predict combustion flame behavior. It is anticipated that the application of ML techniques will eventually reduce computational expenses significantly without having to sacrifice accuracy.

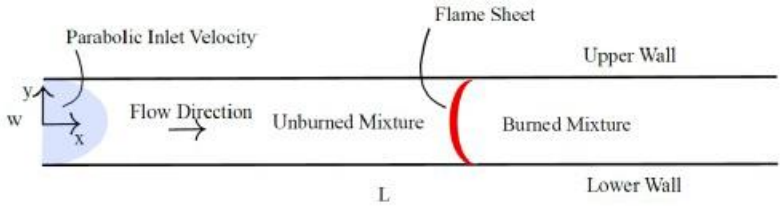


Figure 1: Schematic of the simulation domain

In this work, premixed combustion of two fuel mixtures at stoichiometric level ($\emptyset = 1$) and two different inlet velocities are simulated at micro scale channels (see Figure 1) with detailed chemistry. Details about the operating conditions for these cases are presented in Table 1. Here, w = 2 mm and L = 20 mm are the width and length of the channel, respectively. The simulation domain has the width of 1 mm with an axis-symmetric boundary condition on the lower wall.

Table 1: Variations of fuel mixture and inlet velocity for the selected cases

Case Number	Fuel Mixture	Inlet Velocity (m/s)
Case 1-1	30% CO, 5% CH_4, 65% H_2	1
Case 2-4	40% CO, 10% CH_4, 50% H_2	4

The simulation data, including flow and chemical properties at all grid cells in the computational domain, is separated into two sections: the first section with the largest amount of data (80% of the data) is used to train a Feedforwarding Artificial Neural Network (ANN) model, and the remaining 20% of the data is used to test validate the predictive capabilities and the robustness of the data-driven model.

The ANN model is tested by predicting simulation results at selected time steps that are not seen in the training procedure. Results indicate that it is plausible to train physics-based machine learning algorithms to predict reactive flows with significant reductions in simulation costs. For example, Figure 2 illustrates temperature distribution in the computational domain for Case 2-4 at time 8 ms, where direct numerical simulation (DNS) results are compared with those predicted by the data drive proxy (DDP) model.

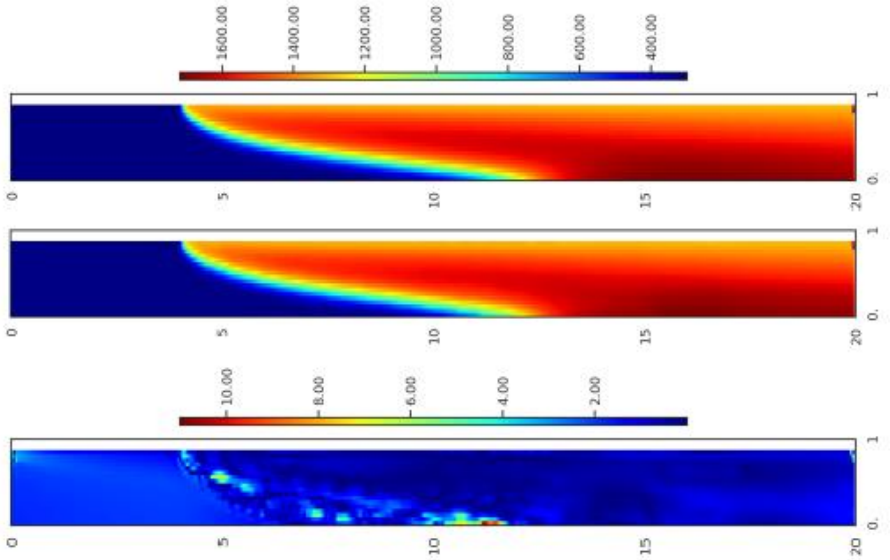


Figure 2: Comparison between temperature (K) predictions via DNS and DDP (Case 2-4 at time t = 8 ms). DNS (top), DDP (middle), and Errors % (bottom)

Results from this work illustrate an overall agreement between predictions from the DDP model and the DNS data. However, there are discrepancies to be addressed. These discrepancies are more considerable at the flame front, where the gradients are larger. For example, heat release rate and temperature experience a very large gradient across the flame front. With providing information about these gradients into the training procedure, such deviations can be reduced in future studies.

Comparisons of direct numerical simulation and penalized models to compute the flow in a porous-fluid system

Charles-Henri Bruneau [1], Didier Lasseux[2], Francisco Valdés-Parada[3]

[1]Univ. Bordeaux IMB, INRIA MEMPHIS, CNRS UMR5251, Talence 33405, France

bruneau@math.u-bordeaux.fr

[2]Univ. Bordeaux I2M, CNRS UMR5295, Talence 33405, France

[3]UAM , Mexico D.F. 09340, Mexico

For more than fifty years now, numerous analyses have been dedicated to the modeling of a porous medium-fluid system, either deriving a boundary condition at the interface or using a simplified model within which the porous medium is taken into account using a penalization method in order to avoid numerical simulation of coupled equations in the fluid and in the porous medium without knowing the appropriate conditions at the interface.

In this work, the porous medium is a large rectangle made of many particles close to each others and the aim is to compute accurately incompressible flow inside and outside the porous medium. The flow is first computed by solving the Navier-Stokes equations in the fluid domain. In a second step, the porous zone is replaced by an homogeneous medium taking into account its properties. Several models are proposed adding a penalization term inside the momentum equation and results are compared to those obtained by direct numerical simulation.

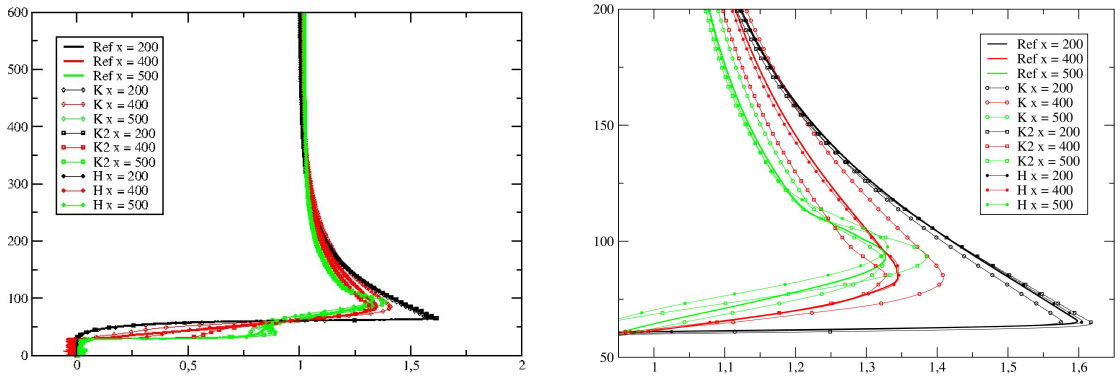
The Navier-Stokes equations are approximated by an accurate finite differences scheme and solved by a multigrid procedure involving several grid levels. The code is highly parallelized with MPI directives.

The models and the results are carefully analyzed to see which penalized model yields results closest to those obtained by the direct simulation. In particular the flow inside the porous medium is scrutinized and the velocity profiles are provided in the whole domain to highlight the impact of penalization approach close to and far from the porous zone.

To get the penalized models a term $\varepsilon\mu H(U)^{-1}U$ is added to the momentum equation where ε is the porosity of the porous medium, μ is the fluid viscosity and H is a tensor

which can depend on the velocity U. The simplest model (K) is obtained while considering H(U)=kI where k is the intrinsic permeability of the porous medium and I the identity tensor. A second order model (K2) with a quadratic term of the velocity can be easily derived and a more complex model (H) depending on the local Reynolds number and on the orientation of the pressure gradient inside the porous medium, can be used to improve the approximation.

The three models are compared to a direct numerical simulation (DNS) of Navier-Stokes equation in the fluid domain between the solid particles and outside the porous medium rectangle that is immersed in the fluid domain. The results are compared for three regimes: steady flow, chaotic flow and turbulent flow increasing the Reynolds number. The results show that for the two first cases the penalized models give a good approximation but not in the third case. This is due to the strong normal velocity coming in front of the porous rectangle that enters too fast inside the porous medium. Fortunately it is possible to modify the K model taking into account the local velocity inside the porous rectangle to get a very good approximation in turbulent case.



Vertical velocity profiles at three locations in x-direction for Re=100. The three models are compared to a reference flow obtained by DNS computed on a much finer grid.

The penalized models will be presented in details at the conference and a thorough discussion of the results will be conducted to convince the audience of the ability of the penalized models that are much cheaper than the direct numerical simulation.

Machine Learning-based Approach for Predicting Defects under Uncertainty in Sheet Metal Forming Processes

P.A. Prates [1], M.A. Dib [2], N.J. Oliveira [2], A.E. Marques [1], M.C. Oliveira [1], J.V. Fernandes [1], B.M. Ribeiro [2]

[1]Centre for Mechanical Engineering, Materials and Processes (CEMMPRE), University of Coimbra

[2]Centre for Informatics and Systems of the University of Coimbra (CISUC), University of Coimbra

pedro.prates@dem.uc.pt

Recently, there has been an increasing use of Machine Learning (ML) algorithms in a variety of engineering tasks. In fact, the vast majority of true Machine Learning users are not experts in Computer Engineering, Algorithms or Mathematics. They are professionals, often engineers working in other fields such as Mechanical Engineering, who want to make the best use of ML algorithms to solve real problems, to which the more traditional algorithms cannot completely respond.

An ML-based approach is proposed to extract information from a sheet metal forming processes, exposed to some sources of scatter, to enable the prediction of defects. The motivation is to reduce the costs and the time spent in the production of defective sheet metal components, i.e. contribute to improve the industry's efficiency. ML techniques are used assuming that they can build models able to generalize well in unseen data. In this context, an empirical analysis of performance of ML techniques is conducted, considering single and ensemble classifiers. These are trained using datasets populated with numerical simulation results of two sheet metal forming processes: U-Channel and Square Cup. Since these processes present distinct features, different types of defects were considered for each one. Each type of defect is studied separately using a binary classification. Moreover, the datasets are generated for each forming process, for three steels with distinct mechanical properties. For a given type of defect, most single classifiers show similar performances, regardless of the material. The fact that ensemble predictive models present relatively high performances, combined with the possibility of reconciling model bias and variance, offer a promising direction for its application in industrial environment.

On the universality of the Strouhal law for High Reynolds number bluff bodies with flow control

Avraham Seifert [1]

[1]Tel Aviv University

seifert@eng.tau.ac.il

In this paper I shall review recent near wake data obtained from a few flow control experiments related to bluff body flow control. In these experiments the main aim is drag reduction and vortex shedding when present is both a source of drag, but can also be used as an indicator for the success of the flow control effort and for drag reduction success. The relationship between natural vortex shedding and forced actuation is studied in detail from both surface steady and unsteady pressures and near wake velocities. It is shown that the classical Roshko results and scaling holds also for controlled wakes. Frequencies above the natural vortex shedding frequencies, especially with 3D actuation, are very effective for separation control and reduction of both surface pressures and wake unsteadiness, along with drag reduction.

Quantified Relationship between Properties of Fresh Self-compacting Concrete and Workability Test Performance

Sizeng You [1], Ashutosh Bhokare[1], *Chenfeng Li[1]

[1]College of Engineering, Swansea University, UK

* Corresponding author: c.f.li@swansea.ac.uk

Self-compacting concrete, known as SCC, has been continuously growing since its invention in 1980s. This type concrete could flow freely under its own weight, which is the most outstanding character. Nowadays, due to the massive production and wide application, a more accurate and quantified understanding on SCC rheology is highly required. The study on this topic has lasted for decades, and it's accepted that flow behavior of fresh concrete can be captured by Bingham Model. Despite of this consensus, a reliable solution to obtain involved parameters of SCC is still absent. Researchers have tried different methods including the analytical, experimental and numerical solutions[1,2,3], but no agreement is reached yet. Instead, the industry chooses to rely on the indicative measures of some robust workability tests.

To improve this situation, a systematic study by numerical simulation was carried out to investigate the flow performance of fresh SCC in standard workability tests. The tests include slump flow test, V-funnel test, modified-cone outflow test and inverted-cone outflow test. For the parameters of Bingham model, yield stress varies from 10 Pa to 100 Pa, and viscosity varies from 10 Pa•s to 100 Pa•s. Before carrying on mass simulation, models for different workability tests require careful design. To achieve better accurary, structured mesh is applied to all models. The most important work in the setup is to decide the element size, which will affect not only computational efficiency but also the model accuracy. The satisfied element size should pass the convergence check and match the accuracy requirement of certain workability test. Following these chosen setups, a batch of simulations were performed and a large set of data was collected recording the whole flow process of all simulations.

Analysis of this set of data shows that the measures of 4 workability tests vary monotonically with either yield stress or viscosity. Therefore, it's known that the 2 parameters of Bingham Model can be uniquely determined by measurements of two different tests. Following this idea, a specific graph depicting the such unique quantified relationship is designed. Considering that the latter 3 tests all belong to outflow tests, 3 test combinations are chosen for graph plotting including (slump flow test, V-funnel test), (slump flow test, modified-cone outflow test) and (slump flow test, inverted-cone outflow test). It's found that all of the 3 graphs share the same pattern with only scale difference as shown in Fig.1. In the figure, τ_0 denotes yield stress, μ denotes viscosity, D denotes spread diameter of slump flow test and t_n denotes discharge time of V-funnel test. And they are easy to be used in practice. Whatever concrete properties are known or measurements of workability tests are known, values of the other can be quickly located on these graphs.

At last, an application example of this graph is performed by simulating construction of a 6-meter high diaphragm wall. According to in-situ test result, the property variation of placed SCC is determined referring to the corresponding graph. In order to shown construction process, 9 representative parameter combination are chosen. The distribution of 9 type different SCC shows the concrete flow pattern in diaphragm wall, as shown in Fig. 2. In the figure, one colour mean one type of concrete and subfigures are taken from cross setions of this diaphragm wall. The number on each subfigure is the distance from this section to one side of the wall.

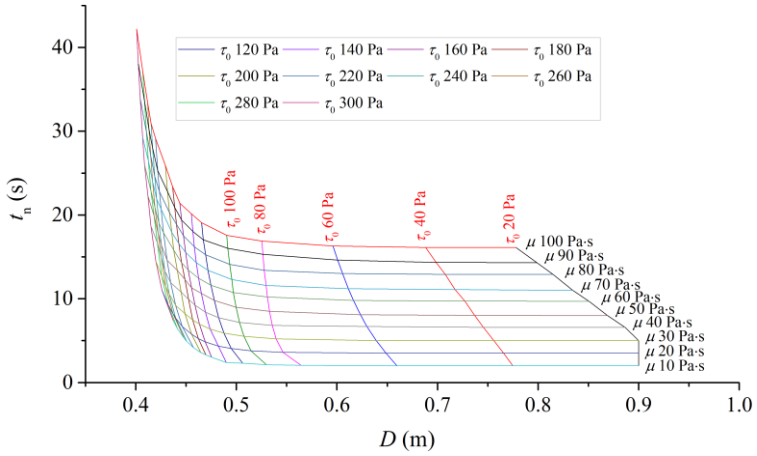


Fig.1 Relationship between (τ_0, μ) and (D, t_n)

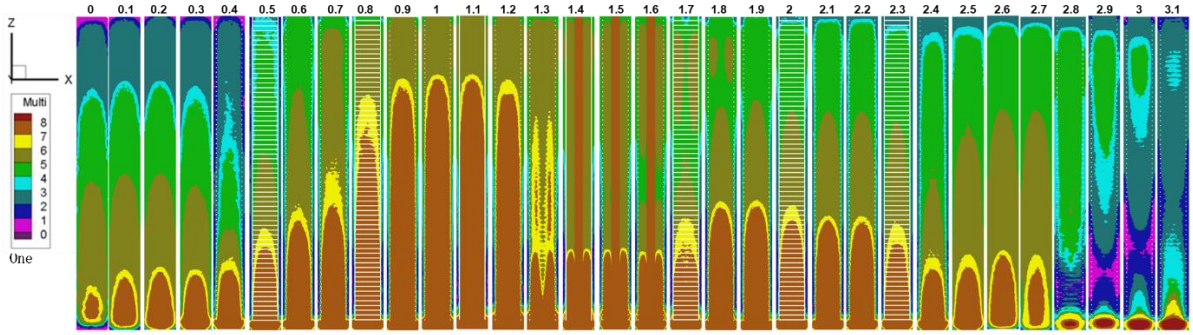


Fig.2 Concrete Distribution in Diaphragm Wall

References

[1] L.E. Brower and C.F. Ferraris. Comparison of concrete rheometers. *Concrete International*, 25(8), 41-47, 2003.

[2] N. Roussel and P. Coussot. Fifty-cent rheometer for yield stress measurements: from slump to spreading flow. *Journal of rheology*, 49(3), 705-718, 2005.

[3] A. Bouvet, E. Ghorbel and R. Bennacer. The mini-conical slump flow test: Analysis and numerical study. *Cement and concrete research*, 40(10), 1517-1523, 2010.

Robust Flame Frequency Response Identification via a Multi-Fidelity Approach

Shuai Guo[1], Camilo F. Silva, Wolfgang Polifke

Technical University of Munich

[1]guo@tfd.mw.tum.de

The frequency response of a linear time-invariant (LTI) system plays a crucial role in the analysis of system dynamics and corresponding system stability. A naive approach to obtain the frequency response of an LTI system is by harmonically exciting the system at many discrete frequencies and obtaining their responses. This method is highly accurate due to the high signal-to-noise ratio (SNR), but is generally not feasible in CFD simulations of complex systems, because of the high computational cost. An alternative method involves broadband excitation combined with advanced system identification analysis. This method, termed SI, provides the complete frequency range of interest of the system response with one single transient simulation. However, the SI method may introduce uncertainties on the identified frequency response due to the limited length of the simulated time series (of the order of tenth of seconds) and the associated low SNR when a strong noise level is present.

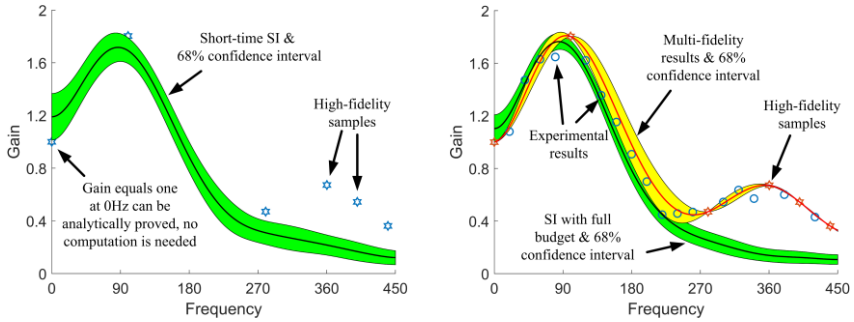
In this study, we propose a multi-fidelity approach to exploit the strengths of the two aforementioned methods to achieve more globally accurate and robust frequency response identification. We aggregate the frequency response identified from a short time broadband excitation (low-fidelity), with responses from harmonic excitations at a few frequencies (high-fidelity). This is realized via *Hierarchical Gaussian Process* (HSP), which takes the low-fidelity results as the global trend in the Gaussian process model of the high-fidelity function. To derive the prediction uncertainty of the multi-fidelity results, firstly, we adopt the regression version of the Gaussian Process, which allows to specify the uncertainties of the high-fidelity training samples and does not enforce interpolation of such samples. In addition, we propose a bootstrapping strategy to propagate the uncertainties associated with the low-fidelity results to the multi-fidelity ones. Since contributions from both fidelities are faithfully taken into account, a robust estimation of the prediction uncertainty of the final multi-fidelity results can be obtained.

This approach is applied here to identify the flame frequency response (FFR). The FFR describes the linear response of a flame to upstream flow perturbations, and

encapsulates the multi-scale multi-physics features of the turbulent combustion dynamics. Additionally, FFR plays a crucial role in the prediction, analysis and control of thermoacoustic instabilities, which are frequently encountered during the operation of low-emission gas turbine combustors.

To thoroughly investigate the effectiveness of the proposed multi-fidelity approach, in the first part of our study, we employ a thermoacoustic network model (a low-order model) where a reference FFR is assumed a priori, to simulate a turbulent swirl premixed burner. This allows us to make systematic assessments of the accuracy, robustness and uncertainty performance of the proposed approach. Two noise levels (high and low) are considered in the current study, and our results indicate that the multi-fidelity approach is particularly preferable in the strong noise case, where a biased and uncertain FFR identified from short-time SI can be effectively corrected by harmonic samples. Thus, this leads to a globally accurate FFR with reduced uncertainty level. We also investigate the sensitivity of the multi-fidelity results to the number and location of frequencies for harmonic excitations, and discuss the optimal strategies for choosing those frequencies.

In the second part of the study, we apply the proposed approach to identify the FFR of a turbulent combustor using signals obtained from large eddy simulations. The identified gain values of the FFR are shown in the figures below. One-third of the computational budget is allocated to perform a short-time SI while the rest is used to perform harmonic excitations. Our multi-fidelity approach aggregates both data and the predicted FFR is more globally accurate and robust, thus demonstrating the effectiveness of the proposed approach.



Future work will focus on developing adaptive sampling schemes to determine the optimal frequencies for harmonic excitations, as well as extending the current multi-fidelity framework to identify frequency responses of other LTI systems.

Numerical modelling of the uncertainties in hip prosthesis material parameters

Fatma ABID[1,2], Abdelkhalak EL HAMI[1], Tarek MERZOUKI[3], Hassen TRABELSI[2], Lassaad WALHA[2], Mohamed HADDAR[2]

[1]Laboratory of Mechanics of Normandy (LMN), National Institute of Applied Sciences of Rouen, Rouen, France

fatma.abid@insa-rouen.fr, abdelkhalak.elhami@insa-rouen.fr

[2] Laboratory of Mechanics, Modeling and Manufacturing (LA2MP), Mechanical Engineering Department, National School of Engineers of Sfax, Sfax, Tunisia

hassen.trabelsi@outlook.fr, walhalassaad@yahoo.fr, mohamed.haddar@enis.rnu.tn

[3]Laboratory of System Engineering of Versailles, University of Versailles Saint Quentin in Yvelines, VELIZY, France

tarek.merzouki@uvsq.fr

The prediction of the mechanical behavior of a bone is a challenging process that has been of agreat attention for reserchers in the biomedical field. The properties of the bone changes from one location to another. Two main types of bone tissue can be distinguished. The inner part is a spongy bone that is characterized by a higher porosity, a higher vascularisation and an ability to absorb energy before the fracture. This type of bone is called cancellous bone. The output bone is characterized by a compact bone. It is called the cortical bone. The composition and the structure of the bone affect its material parameters. However, the composition depends on the nutrition, the disease and the mechanical properties. Kopperdahl and Kevery [1] presented an experimental investigation of the bovine and human specimens. The experiments show that the Young's moduls is related to the bone density. In [2] , the authors study the relationship between the mechanical characteristics and the ash density for the cancellous bone. Kharmanda [3] studied the reliability of a hip prosthesis using a formation material properties. Kharmanda et al. [4] integrate also the multi objactive optimization into an imroved cementless hip prostheis design.

It is worth montioning that the numerical study of such bio mechanical system without taking into account the uncertainties of different parameters has shown a great attention. However, In reality, material parameters show variability and randomness. As a result, the input variation is translated to the output response. Consequently, it is important to carry out an uncertainty analysis that estimates the uncertainty in the hip prosthesis response from the uncertainty in the design variables [5]. In this work, the material parameters are taken as random variables and their influence on the response of the hip prosthysis have been analyzed.

In the literature, we can classify the methods for uncertainty analysis in three main categories: probabilistic methods, non probabilistic methods and analytical methods. Currently, there is a great attention to the probabilistic methods. Among these probabilistic methods, the most frequently used is the Monte Carlo method. This method is widely used due to its robustness and its easy implementation. Nevertheless, the number of achievements must be sufficient. So that, 10^5 or 10^6 deterministic finite element

simulations should be performed to obtain accurate results. The FEM simulation of the hip prosthesis is a complex problem. It takes more time to achieve simulations than a simple problem. Thus, the analysis of the uncertainty using Monte Carlo method will need a large computational time. The spectral stochastic approaches is also a solution for stochastic problem. This method uses a series expansion in order to model a relationship between the uncertainty of the input and thoutput variability. The generalized polynomial chaos (gPC) is considered as one of the spectral stochastic methods. This approach is more efficient to other uncertainties methods. The computational efficiency supplied by the polynomial chaos method is highlited through scientific works in many fields such as solid mechanics [6], fluid dynamics [7] and chemical reactions [8].

The originality of this paper is the increase of the robustness of the hip prosthesis that will operate in presence of uncertainty parameters associated with material properties.

The stochastic approaches described above are coupled with the finite element of hip prosthesis system. A methodology for considering uncertainty in bone materials for a hip prosthesis system is described. The proposed approach is used in order to determine the response of this system with uncertainty related to material parameters. The simulations results are obtained by the generalized polynomial chaos (gPC) method. The proposed technique is an efficient probabilistic tool for uncertainty propagation. It is well shown that the gPC technique is an attractive alternative to the variability studies. For more accuracy, the generalized polynomial chaos results are compared with Monte Carlo simulation.

References

[1] David L Kopperdahl and Tony M Keaveny. Yield strain behavior of trabecular bone. Journal of biomechanics, 31(7):601–608, 1998.

[2] JH Keyak, IY Lee, and HB Skinner. Correlations between orthogonal mechanical properties and density of trabecular bone: use of different densitometric measures. Journal of biomedical materials research, 28(11):1329– 1336, 1994.

[3] G Kharmanda. Reliability analysis for cementless hip prosthesis using a new optimized formulation of yield stress against elasticity modulus relationship. Materials & Design (1980-2015), 65:496–504, 2015.

[4] G Kharmanda. Integration of multi-objective structural optimization into cementless hip prosthesis design: Improved austin-moore model. Computer methods in biomechanics and biomedical engineering, 19(14):1557– 1566, 2016.

[5] Dammak, K., Koubaa, S., El Hami, A., Walha, L., & Haddar, M. (2019). Numerical modelling of vibro-acoustic problem in presence of uncertainty: application to a vehicle cabin. Applied Acoustics, 144, 113-123.

[6] Moez Beyaoui, Manel Tounsi, Kamel Abboudi, Nabih Feki, Lassaad Walha, and Mohamed Haddar. Dynamic behavior of a wind turbine gear system with uncertainties. Comptes Rendus Mecanique 344(6):375–387,2016.

[7] Tonkid Chantrasmi, Alireza Doostan, and Gianluca Iaccarino. Pad´e–legendre approximants for uncertainty analysis with discontinuous response surfaces. Journal of Computational Physics, 228(19):7159–7180, 2009.

[8] Habib N Najm, Bert J Debusschere, Youssef M Marzouk, Steve Widmer, and OP Le Maˆıtre. Uncertainty quantification in chemical systems. International journal for numerical methods in engineering, 80(6-7):789– 814, 2009.

Multi-scale Numerical Simulation of Reinforced Concrete Framed Structure

Tongji University

Prefabricated concrete structures can satisfy the implementation of industrialization and green buildings. Owe to their economic efficiency, less climatic impact, reliable product quality, short construction period and low environmental pollution, prefabricated concrete structures, especially framed structures, have been widely developed in China. The performance of the beam-column joint is the key issue which can affect the seismic performance of the whole structure. Experimental research and multi-scale numerical simulation analysis of cast-in-place frame joints and three kinds of assembled beam-column joints are carried out in this paper.

The experimental study of cast-in-place beam-column joints and three new types of fabricated beam-column joints, which are steel connection joints, sleeve joints and improved steel connection joints, are carried out under low-cycle reversed loading. The comparison of test results shows that the hysteretic curves of steel connection joints is more plump, while possess the best ultimate bearing capacity and energy dissipation capacity.

The shear stress-strain hysteretic relation of cast-in-place beam-column joints was simulated by the micro-scale finite element and the macro-scale element realized by using Joint2D unit in OpenSees while the shear deformation of joint area was considered. The simulated results are in agreement with each other. Due to the complexity of the fabricated steel connection beam-column joints, the micro-scale model will be inefficient to simulate the frame structure design for its complexity. The steel connection joints were simulated by macro-scale joint2D unit to get the shear stress-strain relation skeleton curves while the key parameters such as equivalent elastic modulus of concrete and yield strength of rebar were identified by the two-dimensional space point scatter method which is confirmed by the experimental results.

After that, the cast-in-place frame structure is constituted by the in-suit beam-column joints, and meanwhile, a fabricated frame structure is formed based on the connection manner of the steel connecting joints. . Both of the two frame structures

Formatted: Indent: First line: 0 ch

have six floors and three spans. The reinforcement and dimension of the beam and column for the two framed structures are same, while the joints are different. The whole frame structure is analyzed by the software OpenSees and the joint area was modeled by the macroscopic monolithic joints model. The dynamic time-history analysis of the two frame structures was conducted under the excitation of El Centro wave and the peak acceleration of earthquake motions in elastic and elastic-plastic dynamic time-history analysis is 0.7m/s^2 and 4m/s^2, respectively, which represent the fortification intensity of 8 degrees in China.

For shape steel-connected prefabricated framed structures, the simulated results show that the maximum story drift of the second floor is 4 mm during elastic stage and the inter-story drift ratio is about 1/825. At the elastic-plastic stage, the maximum story drift is 28mm on the first floor, and the inter-story drift ratio is about 1/117. Both the inter-story drifts are smaller than the limit of the inter-story drift at the elastic stage and the elastic-plastic stage, respectively. That meets the design principle of building with no damage under “frequent earthquakes” and no collapse under “major earthquakes”. Therefore, the prefabricated frame structure connected in this way is a feasible connection style. Based on the accuracy of the calculation, the simplified macroscopic joint area model can be used to improve the computational efficiency. This can provide an effective analysis approach for the numerical simulation of the prefabricated framed structures.

Multiscale Moddeling of Self-Affine Rough Contact

A. M. Couto Carneiro[1], R. Pinto Carvalho[1] and F. M. Andrade Pires[1]

[1]Institute of Science and Innovation in Mechanical and Industrial Engineering

{amcc, rcarvalho, fpires}@fe.up.pt

It is well known that, under certain magnification, all surfaces are rough. This has a great impact on many phenomena, such as contact friction, wear, adhesion, thermal behavior and sealing. Moreover, rough surfaces are classified as self-affine, i.e. the roughness features can be observed throughout many scales, down to the nanoscale. The numerical simulation of rough contact, thus, would require prohibitive fine discretization, in order to incorporate all relevant roughness scales.

In this contribution, contact of rough surfaces is analysed using a multiscale finite element framework. Firstly, from a given statistical and spectral surface properties, artificial roughness and profiles are synthesized, by employing a well established non-Gaussian topography generation algorithm [1]. Then, Finite Element meshes are generated from the artificially generated topography, adopting a strategy to reduce, in an orderly fashion, the number of elements with increasing distance to contact regions. Finally, a fully non-linear Finite Element algorithm coupled with a dual mortar contact modelling technique is embedded in a contact homogenization framework [2]. This approach is then used to investigate the effect of the self-affinity of topography on the evolution of the real contact area, comparing the results with analytical models available in literature [3].

[1] Wu, J. J., 2004. Simulation of non-Gaussian surfaces with FFT. Tribology International, 37, 339-349.

[2] Stupkiewicz, S, 2007. Micromechanics of Contact and Interphase Layers. Springer, Verlag Berlin Heidelberg.

[3] Greenwood, J. A. and Williamson, J. P., 1966. Contact of nominally flat surfaces. Proc. R. Soc. Lond. A Math, 295, 300-319.

Presenting Author

Multi-scale adaptive unstructured mesh predictive modelling for environmental problems [1,2,3,4,5]

F. Fang[1*], H. Rong[1], J. Zheng[2], J. Li[3], P. Salinas[1], D. Xiao[4], N.D. Sto. Domingo[5], O. Mark[5], C.C. Pain [1]

[1]Department of Earth Science and Engineering, Imperial College London

[2]Institue of Urban Environment, CAS, China

[3]Institue of Atmospheric Physics, CAS, China

[4]Swansea University

[5]DHI, Denmark

f.fang@imperial.ac.uk

Since multi-physics problems (e.g. coupling of air flow with radiation and chemical reactions for air pollution and atmospheric models) typically have important dynamics that operate over a range of length scales it is necessary to combine these multi-scale methods with multi-physics modeling within the next generation of unstructured mesh models. This provides several profound and widely acknowledged advantages, including: the ability to conform accurately and efficiently to complex domain geometries (for example atomosphere with its geology, an ocean bathymetry or air pollution and flooding a complex cityscape); the ability to dynamically focus resolution and thus focus limited computational resources where it is most required (on areas of particular interest or importance to the dynamics) and simultaneously move the mesh and change the elements/size and shape as well as adapt the order of the accuracy to provide unrivalled numerical resolution/accuracy; and finally, to do all of this in response to the specific modelling needs of the user, while allowing quantitative statements regarding model errors and accuracy to be made. The predictive modelling framework will help determine where discretization and model errors come from and enable us to optimally change our model resolution (e.g. adapt the finite element mesh). The use of adaptive unstructured enables us to resolve physics on a very wide range of spatial scales.

1. Numerical case 1: adaptive mesh modelling in flooding prediction

First, we demonstrate the capability of adaptive meshes in flooding prediction. Over existing adaptive mesh refinement methods (AMR, locally nested static mesh methods),

this adaptive unstructured mesh technique can dynamically modify (both, coarsening and refining the mesh) and adapt the mesh to achieve a desired precision, thus better capturing transient and complex flow dynamics as the flow evolves. Two flooding scenarios are used to assess the performance of a newly developed adaptive mesh flood model (Floodity): the Glasgow's urban flooding event of 2002 and the joint flooding events in Greve, Denmark. The results with use of adaptive meshes have been compared to those from existing models. It has been found that Floodity is able to provide relatively accurate results while the computational cost is reduced by 20 - 88% in comparison to fixed mesh models.

2. Numerical case 2: adaptive mesh modelling in atmospheric and air pollution

Further application of adaptive unstructured mesh is the simulations of air pollution. Once air pollutants are emitted into the atmosphere, the dynamic and chemical processes would transport and transform them continuously. The interactions between these processes involve a wide range of scales. The highly disparate scales pose a formidable challenge for atmospheric and air pollution modelling. In this work, we introduce a new multiscale model for atmospheric and air pollution prediction and controls. The advantage of the adaptive unstructured mesh model has the ability to adapt the mesh according to the evolving pollutant distribution and flow features. That is, the mesh resolution can be adjusted dynamically to simulate the pollutant transport process accurately and effectively. We have successfully applied this new model to a real-life scenario in China – simulated the pollutant released from over 100 coal power plants across 55 cities including Beijing.

3. Machine learning and reduced order modelling

We present new numerical techniques such as, machine learning (ML), reduced order modelling (ROM) and data assimilation (DA), for real-time operational modelling and uncertainty analysis. Having the compatibility of both ML and ROM will be nothing short of revolutionary for a large number of disciplines. Here the capabilities of ML-ROMs have been demonstrated in air pollution, urban flows, ocean, flood prediction. The combination of ROM, ML and DA enables a rapid and accurate modelling response in emergencies.

A Global-Local Zooming Technique

Matthias Birner[1], Marc Alexander Schweitzer

[1]Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI

matthias.birner@scai.fraunhofer.de

In this talk, we present a novel zooming scheme based on global-local enrichments, to tackle multi-site damage problems in laminated composites.

Typically, a classical FEM requ1ires a very large number of degrees of freedom to resolve fine-scale features, as cracks in fracture mechanics problems. Partition of unity methods, as e.g. the GFEM, XFEM or PUM can circumvent this computational overhead by employing problem specific basis functions, so called enrichments. Unfortunately appropriate enrichments are only known analytically or a-priori for a few application cases. Duarte et al. proposed a global-local enrichment method to compute simulation specific enrichments on the fly. Based on this approach we present a zooming scheme that further condenses degrees of freedom and can handle multiple scales present in a problem.

We present numerical results in 2D for laminated composites which show several delamination zones. Here, an essential ingredient is the use of a new set of analytic enrichment functions for bi-material interfaces based on those by Sukumar et al.

C. A. Duarte, D.-J. Kim, and I. Babuška, A global-local approach for the construction of enrichment functions for the generalized fem and its application to three-dimensional cracks, Advances in meshfree techniques, Springer, 2007, pp. 1–26.

N. Sukumar, Z. Y. Huang, J.-H. Prévost, and Z. Suo, Partition of unity enrichment for bimaterial interface cracks, International journal for numerical methods in engineering 59 (2004), no. 8, 1075–1102.

Multiscale prediction of powder properties during pressure-assisted sintering

Szymon Nosewicz [1*], Jerzy Rojek[1], Krzysztof Wawrzyk[1],

Piotr Kowalczyk[1], Grzegorz Maciejewski[2], Marcin Maździarz[1]

[1]Institute of Fundamental Technological Research Polish Academy of Sciences, Warsaw, Poland
[2]Institute of Aviation, Warsaw, Poland
*snosew@ippt.pan.pl

Sintering is a fundamental technology in manufacturing of new advanced materials with many applications, such an automotive or aerospace. Sintering can be defined as the thermal treatment of a powder (or compact) at a temperature below the melting point of the main constituent, for the purpose of increasing its strength by bonding together the particles. The obtained sintered body has a significantly different form compared to the initial state. When powder compacting and sintering occur simultaneously, it is called a pressure-assisted sintering. The evolution of the sintered powder with external pressure is governed by many factors at different scales. Due to the complexity of the process, the description of the sintering phenomenon is a non-trivial task. Macroscopically during sintering, one can observe changes of the bulk material volume (shrinkage) and, associated with this, densification and decrease of porosity. The microstructure during sintering undergoes an evolution characterized by grain rearrangement, increase of grain compaction and formation of cohesive bonds between powder particles which occurs due to mass transport. Surface and grain boundary diffusion are normally dominant mechanisms of mass transport in sintering.

Such a large number of material effects occurring at several scales during sintering cannot be described comprehensively with a single modeling approach. The macroscopic properties are influenced by several factors at various scale interact with one another, hence in numerical modeling we should take into account material phenomena occurring at different levels. In contrast to the traditional approaches, which focus on one scale, multiscale modeling simultaneously considers models at different scales, sharing the efficiency of the macroscopic models as well as the accuracy of the microscopic models.

Such a multiscale approach explores the advantages of lowest scale calculation, for example, molecular simulations, allowing insight into atomic-scale processes at a short time scale, and macroscopic simulations, allowing simulations at a much longer timescale. Constitutive models at various scales are connected which allows us to perform an investigation of various phenomena occurring at different scales.

Within the proposed work, development of numerical models predicting the powder properties during pressure-assisted sintering has been performed for different scales: atomistic, microscopic and macroscopic one. Varied approaches and varied numerical models adequate for each level have been applied. The molecular dynamics (MD) simulations have been performed to determine the diffusive parameters at the atomistic scale. MD simulations allowed to determine the input parameters of micromechanical discrete element model (DEM). By taking into account the composite microstructure, microscopic model has provided data (density and temperature dependent viscosity of material) for macroscopic modeling (finite element framework). The macroscopic constitutive model is based on the assumption that the sintered material is a continuous medium. The numerical model will be validated by the data obtained within the own experimental research by sintering of NiAl powder.

ACKNOWLEDGMENTS

The results presented in the paper have been obtained within the projects funded by the National Science Centre awarded by decision numbers DEC-2013/11/B/ST8/03287.

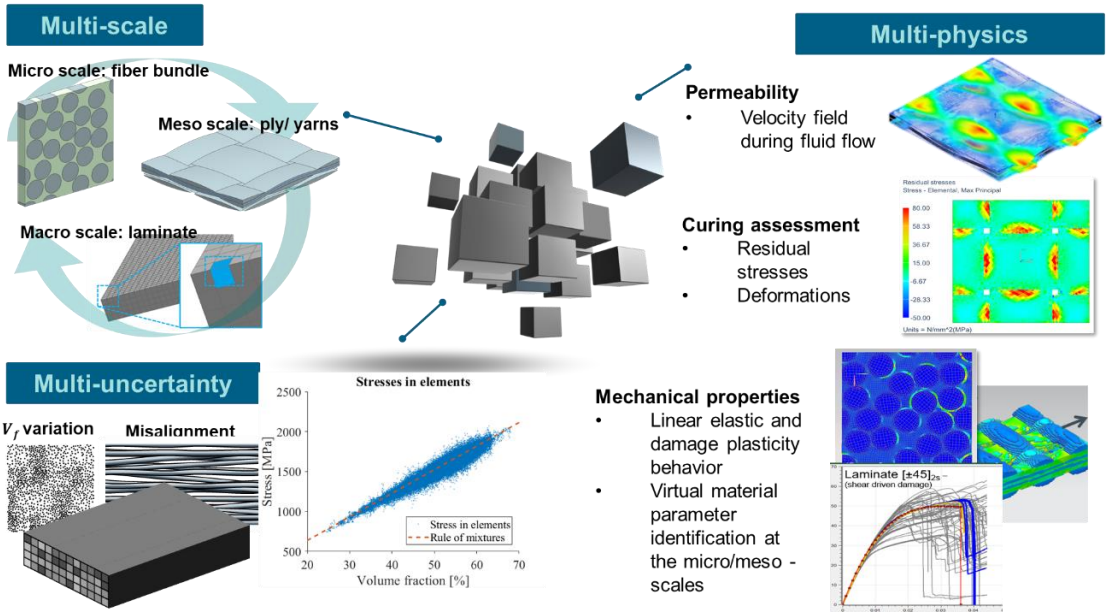
Virtual material characteriazation across scales and physics: case studies

Anna Matveeva, Oxana Shishkina, Fabio Malgioglio, Laszlo Farkas

Siemens Industry Software NV (SISW), Interleuvenlaan 68, 3001 Leuven, Belgium

anna.matveeva@siemens.com

Material engineering for composites is a complex process covering different stages from application-driven design and manufacturing method selection to composite production and performance assessment via iterative optimization loops. Large and expensive test campaign is needed before the final design decision is made. With the Simcenter 3D (Siemens PLM Software) Virtual Material Characterization (VMC), the material engineering process becomes more efficient and can be completed with fewer tests. This contribution demonstrates different stages of a VMC process including solutions for multi-scale, multi-uncertainty and multi-physics problems as depicted in the Figure below.



The modelling workflow of the VMC ToolKit is based on the concept of the representative unit cell (RUC) combined with sequential homogenization schemes for the scale transition. Different material scales and a wide range of supported fiber-reinforced composite types are covered including both, idealized CAD representation and realistic micro-CT-based voxel models.

Three case studies are elaborated in this work. 'The multi-scale' study case focuses on the scale transition for multidirectional laminates. Reverse-engineering of the nonlinear behavior of constituents on the micro-scale is discussed, followed by a virtual parameter identification for the meso-scale ply damage model developed in LMT-Cachan (Ladevèze et al., 1992). 'The multi-physics' cases are linked to the manufacturing simulations. The effect of curing on the development of residual stresses and deformations is studied in thermosetting composite materials on the micro-scale. In order to gain insight into the infusion process, saturated permeability is computed for woven composite RUCs (meso-scale) and first steps towards unsaturated permeability assessment on the micro-scale are discussed. 'The multi-uncertainty' case focuses on the effect of the material variability by the example of a unidirectional composite (UD). The longitudinal tensile strength of a UD ply is predicted, considering the stochasticity of the fiber strength and microstructure (misalignment and fiber volume fraction variability).

The demonstrated Simcenter 3D VMC ToolKit, with a link to micro-CT images, permeability calculations, curing simulations, assessment of the variability and virtual material parameter identification across different material scales, provides an industrial solution for the efficient linking of the manufacturing-induced material features to the materials' performance.

Acknowledgement:

The authors gratefully acknowledge SIM (Strategic Initiative Materials in Flanders) and VLAIO (the Agency Flanders Innovation & Entrepreneurship) for their support of the ICON project M3Strength (Grant no.140158), which is part of the research program MacroModelMat (M3), coordinated by Siemens Industry Software (SISW). O. Shishkina thanks VLAIO for financing her work in the framework of the Innovation Mandate Project "MicroCT-based Model Generation Engine for Virtual Material Characterisation" (Grant no. HBC.2017.0189). F. Malgioglio thanks the EU Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 722626 for funding his work through the FiBreMoD project and his supervisors Prof. S.V. Lomov, Dr. Y. Swolfs, Prof. W. Desmet (KU Leuven, Belgium). The Mechanics of Materials and Structures research group (Ghent University, Belgium) coordinated by Prof. W. Van Paepegem is acknowledged for the support. We thank H. Egami (University of Tokyo, Japan) for his contribution to the research on unsaturated permeability during his internship at SISW through the program "Vulcanus in Europe" by EU-Japan Centre for Industrial Cooperation. We also thank G. Romano (University of Calabria, Italy) for performing study on curing in the scope of the Master thesis internship at SISW.

Heat transfer partitioning models for nucleate boiling

Robin Kamenicky [1], Michael Frank [1], Dimitris Drikakis [2], Konstantinos Ritos [1]

[1]University of Strathclyde, Glasgow, United Kingdom

[2]University of Nicosia, Nicosia, Cyprus

robin.kamenicky@strath.ac.uk

Nucleate boiling is relevant to several industrial sectors, e.g., metallurgy (quenching in manufacturing) and nuclear reactors. Despite considerable efforts [1, 2], the development and validation of nucleate boiling models remains an active field of research.

An essential part of nucleate boiling modeling is the treatment of the (boiling) boundary condition. This paper focuses on heat transfer partitioning models. The efficacy of partitioning models to accurately predict heat transfer depends on the choice of auxiliary models that describe nucleation site density, bubble detachment frequency, and bubble detachment diameter. Various models for specific applications have been proposed [3]. Their applicability depends on the range of pressure, water subcooling, and mass flow rate values. Most of these models were developed for operational conditions in nuclear power reactors. However, there is a number of low pressure, high subcooling applications, such as metallurgical quenching or high power electronics that would benefit from further development.

Although the Kurul & Podowski model [4] is widely used, its robustness and accuracy is questionable. Gilman et al. confirmed the robustness issue, when their numerical prediction suffered from divergence at high heat fluxes [5]. Alternative models have also been proposed [5-7]. Apart from evaporation, quenching and convection heat transfer, the new models account for other heat transfer phenomena such as heat transfer caused by sliding bubbles or the effect of a microlayer. In this paper, various heat transfer partitioning models in conjunction with a conjugate heat transfer boundary condition for the fluid-solid interface, are assessed numerically. The implementation is into the OpenFOAM CFD software. The physics within the solid is modelled using an energy equation, whereas the fluid flow domain is modelled by the Navier-Stokes equations for the vapour and liquid phases.

The models are firstly compared against original experiments used for their development by their authors. This allows to verify proper code implementation. Then the partitioning models are compared using common experiment.

[1] Ilić, M. M., Petrović, M. M., Stevanović, V. D., Boiling Heat Transfer Modelling: A Review and Future Prospectus, Thermal Science, Vol. 23, No. 1, pp. 87-107, (2019).

[2] Chapter 2 - Nucleate Boiling. In: Boiling. Ed. by Yasuo Koizumi et al. Boston: Elsevier, pp. 13–144, (2017).

[3] Cheung, S. C. P., Vahaji, S., Yeoh, G. H., Tu, J. Y., Modeling subcooled flow boiling in vertical channels at low pressures – Part 1: Assessment of empirical correlations, International Journal of Heat and Mass Transfer, pp 736–753, (2014).

[4] Kurul, N., Podowski, M.Z., On the modeling of multidimensional effects in boiling channels, ANS. Proc. National Heat Transfer Con. Minneapolis, Minnesota, USA, pp. 30-40, (1991).

[5] Gilman, L., Baglietto, E., A self-consistent, physics-based boiling heat transfer modeling framework for use in computational fluid dynamics, International Journal of Multiphase Flow, pp 35–53, (2017).

[6] Basu, N. , Gopinath, W., Dhir, V.K., Wall Heat Flux Partitioning During Subcooled Flow Boiling: Part 1—Model Development, Journal of Heat Transfer transactions of The Asme - J HEAT TRANSFER (2005).

[7] Yeoh, G. H., Vahaji, S., Cheung, S. C. P., Tu, J. Y. Modeling subcooled flow boiling in vertical channels at low pressures – Part 2: Evaluation of mechanistic approach, International Journal of Heat and Mass Transfer, pp 754–768, (2014).

A fully coupled electromagnetic-thermal-transient mechanical simulation of the load suffered by aeronautical composite panels during lightning strikes

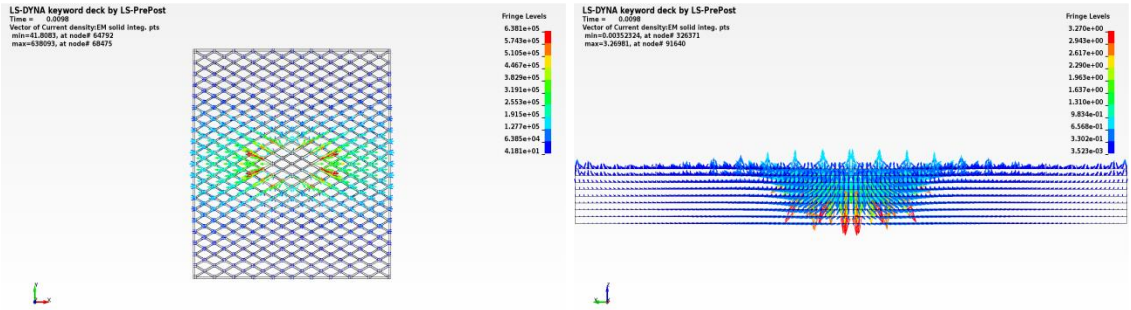
Christine Espinosa [1], Fabio Martarelli [1], Frédéric Lachaud [1]

[1] Institut Clément Ader, Université de Toulouse, ISAE-SUAPERO, IMT MINES ALBI, UTIII, INSA, CNRS, 3 Rue Caroline Aigle, F-31400 Toulouse CEDEX 04, France

christine.espinosa@isae-supaero.fr frederic.lachaud@isae-supaero.fr

One of the main multi-physical and multiscale safety issues facing aircrafts is the protection against lightning strikes. Because of the low electrical conductivity of composites compared to metal, composite aircrafts must be protected against current flows. It is done by metallic mesh coatings. Tests done at AIRBUS showed that when protected by appropriate metallic meshes, composite panels do not delaminate anymore [1]. It has been demonstrated that delamination is mainly due to a resultant mechanical impulse transmitted to the composite panel by the multi-physical phenomena in the protection layers [2, 3, 4]. In presence of paint, the vaporization process is replaced by an explosion which causes delamination [1, 5, 6]. Observed damages in protected GFRP and CFRP or unprotected CFRP panels suggest that the vaporization of the resin of the upper ply of carbon fiber reinforced composite make possible current injection in the composite fibers which causes the explosion [6]. It is thus of primary importance to evaluate the contribution of the different physical components of the lightning strike on the load transmitted to the composite panel, and if the composite is part of its loading.

This talk will present the strategy proposed to model the fully coupled multi-physics behavior of a protected aeronautical panel during the injection of a D-wave current mimicking lightning. A previous coupled FE model allowed us to compute the stress, temperature and current distribution resulting from injection of a D-waveform using a simplified model for the metallic mesh and an evolving injection zone [7]. The predicted mechanical impulse was of the order of magnitude of pressures estimated by energy models [2, 4], but the coarse FE mesh was responsible of oscillations in the Joule resulting temperature and in the pressure. In the present model the FE mesh of the metallic protection is refined and connected to the composite plate through a mechanically thermally and electrically continuous contact. It is shown that current and impulse are indeed the most important load components transmitted to the composite.



Current distribution in the mettalic mesh (left) and the composite panel (right)

[1] A. Bigand, C. Espinosa, J.M. Bauchire, F. Flourens, F. Lachaud (2018). Estimation of the load produced by the electro-thermal behavior of lightning strike protection layers on a composite panel. 18th European Conference on Composite Materials (ECCM18), Athens, Greece.

[2] F. Soulas, C. Espinosa, F. Lachaud, S. Guinard, B. Lepetit, I. Revel, Y. Duval (2018). A method to replace lightning strike tests by ball impacts in the design process of lightweight composite aircraft panels. International Journal of Impact Engineering, 111, 165-176.

[3] A. Bigand, C. Espinosa, H. Rabat, J.M. Bauchire (2018). Lightning strike protection explosion and overpressure profile. 15th High-Technology Plasma Processes (HTPP15), Toulouse, France.

[4] C. Karch, A. Arteiro, P. Camanho (2019). Modelling mechanical lightning loads in carbon fibre-reinforced polymers. International Journal of Solids and Structures, 162, 217-243.

[5] A. Bigand, J.M. Bauchire, C. Espinosa (2018). Lightning arc interaction with complex structure. 15th High-Technology Plasma Processes (HTPP15), Toulouse, France.

[6] A. Bigand, Y. Duval (2017). Quantification of the mechanical impact of lightning strike protection explosion confined by thick paint. International Conference on Lightning and Static Electrocity (ICOLSE), Nagoya, Japan.

[7] C. Espinosa, T. Montel, J. Montes Pons, F. Lachaud, F. Soulas (2017). A numerical study of the pressure applied on CFRP panels during a lightning strike using a coupled electro-thermal-mechanical model. International Conference on Lightning and Static Electrocity (ICOLSE), Nagoya, Japan.

Modelling of shear bands in fluid saturated poroplastic solids with embedded strong discontinuities

Mijo Nikolic[1], Adnan Ibrahimbegovic[2]

[1]University of Split, Faculty of Civil Engineering, Architecture and Geodesy, Split, Croatia

[2]Université de Technologie de Compiègne/Sorbonne Universités, Laboratoire Roberval de Mécanique, Compiègne, France

mijo.nikolic@gradst.hr

Simulations of shear bands require special treatments due to its localized nature. Namely, localized failure is mesh-dependent when standard finite element method is used. Various methods have been developed to tackle this difficulty. However, it is still challenging to be able to simulate this problem in complex environments, such as porous heterogeneous medium with multiple phases and where we could have multiple shear band developments interacting with each other. The presence of fluid inside such medium brings additional complexities. In this work, we present the way to compute such problem in efficient way. The framework for considering multi-phase material with multiple shear bands is based on lattice element method, while pathological mesh dependence with localized failure is eliminated by using embedded strong discontinuities inside elements. No global tracking procedure is required in this approach which also enables easier propagation of multiple bands and their interaction. Moreover, computational algorithms are efficient due to such strategy. Additional strength of the algorithm is that embedded discontinuities are computed at element level and no additional degrees of freedom for existence of localized failure are required. Presence of fluid and its influence to shear band forming is provided with Biot poroelastic approach. Here, we consider material to be plastic with microcracks prior to localized shear band forming. The Darcy law is used to compute fluid flow inside the poroplastic domain.

Acknowledgements: This work has been supported by the Croatian Science Foundation under the project number UIP-2017-05-3429

Comparison of Two New Methods for Fatigue Reliability Analysis

Ruofan Gao[1], Jie Li[2]

[1] School of Civil Engineering, Tongji University, Shanghai, China

gaoruofan529@gmail.com

[2] School of Civil Engineering and the State Key Laboratory on Disaster Reduction in Civil Engineering, Tongji University, Shanghai, China

lijie@tongji.edu.cn

With a review of the previous researches, the traditional fatigue reliability analysis methods are divided into two types, namely, the S-N curve-based methods and the fracture mechanics-based methods. However, both kinds of methods have their limitations. The S-N curve methods lack university, and can hardly indicate the damage development. The fracture mechanics-based models mainly focus on the single macro crack, and cannot reflect fatigue damage state before the formation of the macro crack.

Based on continuous damage mechanics (CDM) and probability density evolution theory (PDEM), this paper develops two new fatigue reliability analysis methods, and compares these two analysis methods from different perspectives. The first new method is based on the remaining fatigue life. Based on the CDM, a stochastic fatigue damage model is introduced for the deterministic structural analysis, by which the fatigue damage process of structure is derived. According to the PDEM, the probability density evolution equation for the remaining fatigue life is built to perform the stochastic analysis. By solving the probability density evolution equation, the probability density function (PDF) of the remaining fatigue life evolving with time is obtained. The fatigue reliability is finally calculated by integrating the PDF of the remaining life. The other new method is the physical synthesis method. The physical equations of solid mechanics are determined by using the stochastic fatigue damage model. Based on the fatigue damage-based failure criterion, the physical synthesis method is developed by combining the physical equations of solid mechanics with the probability density evolution equation. The fatigue reliability is obtained by solving the equations of the physical synthesis method.

The paper compares the theoretical basis of the two new methods for fatigue reliability analysis to illustrate the similarities and differences as well as the advantages

and disadvantages of the two methods. Moreover, the two methods are applied to analyze the fatigue reliability of a concrete continuous beam bridge under random vehicle loading, respectively. The results of fatigue reliability obtained by the two methods are compared in details, to mutually verify the validity of each other and intuitively reflect their advantages and disadvantages.

Construction of optimal basis functions in the Partition of Unity Method and their verification in complex simulations

Denis Düsseldorf [1]

Prof. Dr. Marc Alexander Schweitzer [2]

[1]University of Bonn

[2]University of Bonn and Fraunhofer SCAI

duesseld@ins.uni-bonn.de

In this talk, we present the construction of optimal basis functions for orthotropic laminates with holes that resolve the fine scale details of the solution and the verification of these basis functions in an application setting. The goal of this research is to construct a computational efficient model with very few degrees of freedom, yet approximation properties similar to a fine-scale model so that automatic optimization of layup design and margin of safety assessments including structural details become feasible.

The method is implemented using the Partition of Unity method (PUM), a meshfree generalization of the GFEM or XFEM. The independence of local approximation spaces in the PUM allows us to apply the optimal basis functions in regions where heavy refinement is necessary in the standard methods. We present numerical results in 2D and 3D.

Ivo Babuska and Robert Lipton, Optimal Local Approximation Spaces for Generalized Finite Element Methods with Application to Multiscale Problems, Multiscale Model. Simul., 9(1), 373–406. (34 pages)

A Vibrational study of graphene sheets, carbon nanotubes, and nanocones

Reza Ghaffari [1], Aningi Mokhalingam [2], Shakti S. Gupta [3], Roger A. Sauer [4]

[1,4] Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Templegraben 55, 52056 Aachen, Germany

[2,3] Department of Mechanical Engineering, IIT Kanpur, Kanpur - 208016, India

[1] ghaffari@aices.rwth-aachen.de

[2] aningi@iitk.ac.in

[3] ssgupta@iitk.ac.in

[4] sauer@aices.rwth-aachen.de

In this paper, the frequencies of the transverse vibrations of radially stretched circular graphene sheets, carbon nanotubes, and carbon nanocones are studied comparing atomistic approaches and a new continuum model based on density functional theory data.

The continuum model is nonlinear, hyperelastic, and anisotropic. The strain energy density is written in terms of a set of invariants based on the logarithmic strain and structural tensor [1]. The model is calibrated with density functional theory (DFT) data and implemented in the curvilinear rotation-free finite element formulation of [2]. The employed framework was previously used for the development of membrane and shell material models for graphene [1,3, 4].

In the molecular mechanics simulations, the MM3 potential is used to define the interaction between carbon atoms. The system is first relaxed to the minimum energy configuration. Then, the outer edge atoms are displaced radially untill the required stretch is obtained. The frequencies are found by using the VIBRATE module in Tinker [5].

Molecular dynamics simulations are carried out using REBO+LJ potential in LAMMPS. The minimum energy configuration is equilibrated using a Nose-Hoover thermostat at 0.1 K. Three Nose-Hoover chains are employed to maintain the temperature of the system at the desired level. After pulling the outer edge of the atoms up to a desired stretch, the sheet is deformed into the first mode shape and then allowed to vibrate freely while the total mechanical energy of the system is kept constant. The time history of the

atoms at the center is recorded to calculate the frequencies of vibration using a fast Fourier transform (FFT).

Modal analysis of the circular graphene sheets, carbon nanotubes, and carbon nanocones is conducted using the continuum model and compared with the results from molecular dynamics simulations. The variation of the first frequency versus the surface change J is shown in Fig. (1) for a graphene sheet and the results are in good agreement in all three approaches up to J = 1.2. The deviation of the results is larger for J > 1.2 and - due to the breakage of the bonds for J > 1.4 in Rebo+LJ potential - the results are only presented up to this strain.

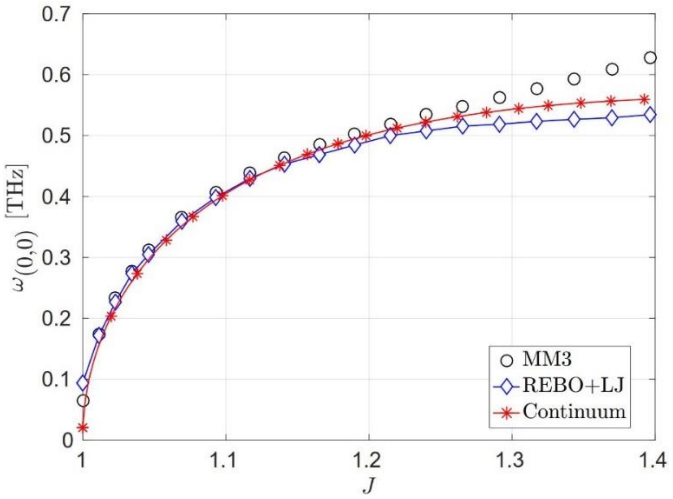


Figure 1: Variation of the first mode frequency versus the surface stretch for a graphene sheet

REFERENCES

[1] Reza Ghaffari and Roger A. Sauer. A new efficient hyperelastic finite element model for graphene and its application to carbon nanotubes and nanocones. Finite Elem. Anal. Des., 146:42-61, 2018.

[2] Thang X. Duong, Farshad Roohbakhshan, and Roger A. Sauer. A new rotation-free isogeometric thin shell formulation and a corresponding continuity constraint for patch boundaries. Comput. Methods in Appl. Mech. Eng., 316(Supplement C):43-83, 2017. Special Issue on Isogeometric Analysis: Progress and Challenges.

[3] Sandeep Kumar and David M. Parks. On the hyperelastic softening and elastic instabilities in graphene. Proc. Royal Soc. Lond. A: Math. Phys. Eng. Sci., 471(2173), 2014. DOI: 10.1098/rspa.2014.0567.

[4] Reza Ghaffari, Thang X. Duong, and Roger A. Sauer. A new shell formulation for graphene structures based on existing ab-initio data. Int. J. Solids Struct., 135:37-60, 2018.

[5] J.W. Ponder. Users guide computer code tinker molecular modelling package 4.2, 2004.

Metamodels for RBDO of wire bonding in microsystem packages

Hamid HAMDANI [1,2] Bouchaïb RADI [2] Abdelkhalak EL HAMI [1]

[1]LMN, Normandie Univ, INSA Rouen, 76000 Rouen, France

[2]LIMII, FST Settat, BP: 577, Route de Casa, Settat, Morocco

hamid.hamdani@insa-rouen.fr, bouchaib.radi@yahoo.fr, Abdelkhalak.elhami@insa-rouen.fr,

For microelectronic device structures, several reliability-based design optimization Methodology (RBDO) was developed. The main objective of such method is to design structures, which should be both economical and reliable where the solution reduces the structural weight in uncritical regions. It does not only provide an improved design, but also a higher level of confidence in the design. This paper focuses on the use of metamodeling technics with high efficiency to overcome the time-consuming of the multiphysics finite element simulation in the RBDO process.

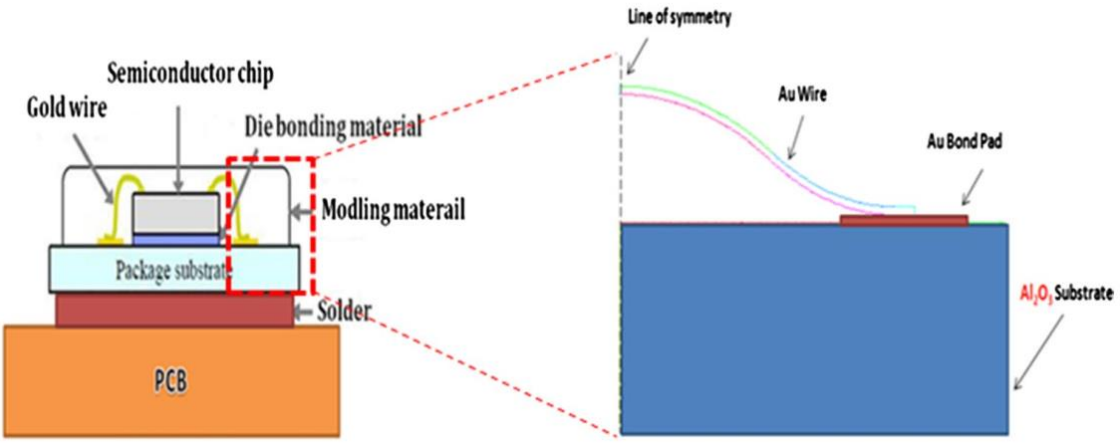


Figure 1: Structure of the electronic package (wire bonding type) and 2D scheme of the model

More precisely, the Finite element simulation model, which intends to analyze the sequence of the failure events in power microelectronic devices, is replaced by appropriate metamodels. The constructed metamodels are validated and compared by cross validation and error measures. Then, the suitable metamodel is chosen according to its quality. The chosen metamodel is used to estimate the probability of failure of power

module. Subsequently the reliability analysis is integrated in the optimization process forming a sequential RBDO algorithm in order to find the best structural designs of wire bonding technologies and to realize the best compromise between cost and safety. The metamodel based RBDO method used in this paper is an approach with high-efficiency and sufficient accuracy. It has improved the traditional methods that use response surfaces without validation.

References

[1] Makhloufi, A., Aoues, Y., and El Hami, A. (2016). Reliability based design optimization of wire bonding in power microelectronic devices. *Microsystem Technologies*, 22(12):2737–2748.

[2] Hamdani, H., Radi, B., and El Hami, A. (2017). Métamodélisation pour une conception robuste des systèmes mécatroniques. *Incertitudes et fiabilité des systèmes multiphysiques*, 2(Numéro 2):10.

[3] Liu DS, Chao YC, Wang CH (2004) Study of wire bonding looping formation in the electronic packaging process using the three-dimensional fnite element method. *Finite Elem Anal Des* 40:263–286

[4] Hamdani, Hamid, Radi, Bouchaïb, and El Hami, Abdelkhalak. Optimization of solder joints in embedded mechatronic systems via kriging-assisted cma-es algorithm. *Int. J. Simul. Multidisci. Des. Optim.* , 10 :A3, 2019.

New Method for Numerical Calibration of a Rotary Kiln Model – A Multiscale Approach

Christian Jordan [1], Mario Pichler [1], Bahram Haddadi [1], Hamidreza Norouzi [2], Florian Wesenauer [1], Jakob Weber [1], Franz Winter [1], Michael Harasek [1]

[1]Institute of Chemical, Environmental and Bioscience Engineering, TU Wien, Getreidemarkt 9/166, 1060 Vienna, Austria

[2]Department of Chemical Engineering, Amirkabir University of Technology, Tehran, Iran

christian.jordan@tuwien.ac.at

Rotary kilns are widely used in industry for the production of a range of products including cement, lime or iron ore pellets and the re-utilization of by-products such as the thermal utilization of solid waste or black liquor in pulp and paper industry. Rotary kilns are also an excellent example of multiple scales: Millimeter sized particles are treated in a device with a characteristic length of several meters.

While there are macroscopic models to describe the global particle movement and filling conditions in a rotary kiln, such as the volumetric fraction of bulk solids, the average residence time or the linear velocity of solids in axial direction, those models provide only a limited amount of information and the validity of the models is typically limited to the calibration space.

For thermal utilization of solid waste not the overall (averaged) residence time, but the residence time of different particle types (material, shape, size) in different zones of the kiln is especially important. Particles are exposed to different conditions (temperatures, gas flow rates, gas composition), along the rotation axis of the kiln - a different combustion and heat- and mass-transfer behavior is expected in each zone.

A detailed simulation of the particle motion in rotary kilns using the Discrete Element Method (DEM) can help to get deep insight in the particle movement and the individual exposure to the kiln environment, the individual residence time profile, as well as particle-particle and particle-wall interactions - however, DEM is computationally expensive. Therefore, DEM simulation data can be used for the calibration of custom-tailored macroscopic models, which are utilized to optimize production processes and equipment in terms of efficiency, product quality and production output and to provide input data for subsequent simulation steps.

In this work experimental investigations and numerical simulations, using the Discrete Element Method, of a lab-scaled rotary kiln have been carried out (see also Figure 1). Focus is the investigation and validation of the residence time of the different particle types in the rotary kiln. The mean residence time and residence time distribution (RTD) in simulation and experiments have been evaluated after reaching a steady state using marked tracer particles. Simulation and experiments show good agreement in terms of mean residence time, RTD and the dynamic angle of repose.

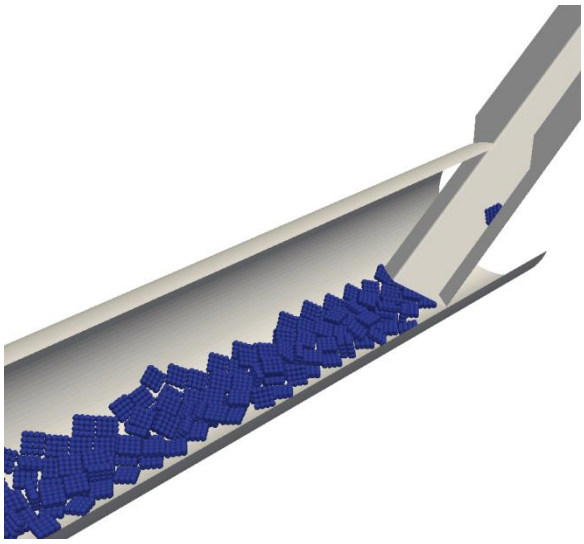


Figure 1 DEM simulation of the lab scale rotary kiln

Using the validated numerical data, the mean residence time profile for each particle type can be calculated for each kiln zone and can then be used for subsequent combustion calculations in 1D or 3D computational fluid dynamics (CFD) models. This combined method is a promising approach for reducing the complexity of the particle movement while keeping relevant information, especially for industrial scaled rotary kilns.

Nanoscience applied to oil and gas technologies: a multiscale computational approach

Caetano R. Miranda [1]

[1]Instituto de Física - Universidade de São Paulo

crmiranda@usp.br

Advances in nanostructured materials have opened a wide range of multifunctional materials with promising potential to control interfaces and flow at nanoscale. Here, I will summarize some of the activities at our group based on multiscale modeling to explore the potential applications of nanoscience for Enhanced Oil Recovery (EOR) processes and fluid flow through nanoporous media. Our strategies are focused on i)Nano-EOR, based on surface drive flow, where mobilisation of hydrocarbons trapped at the pore scale is favored by controlling by the chemical environment through Wetability modifiers and ii)Nano-IOR, through pressure driven flow, by controlling the spatial confinement and fluid flooding at nanoporous. In this hierarchical multiscale protocol, the amount of oil displaced by fluid injection (brine, NP solution, or surfactants) within pore network models (PNMs) is estimated with controlled porosity, size, shape and porous distribution. Initially, the systems of interest are characterized by first principles calculations based on the Density Functional Theory and their atomic interactions validated with interatomic potentials to be used within fully atomistic molecular dynamics (MD)[1-2]. At MD level, the interfacial and transport properties are determined at reservoir conditions. Those properties are mapped into Lattice Boltzmann Method[3] (LBM) parameters to describe the fluid-fluid and fluid-solid interactions. At LBM level, the injection of fluids (brine, NPs and surfactants) is simulated within PNM models previously filled with oil. This can be a useful tool to explore chemical additives for EOR and investigate the wetting effects on fluid behavior and oil displacement in porous media over scales. Applications will be illustrated and the challenges and limitations of this methodology will be discussed.

[1]Miranda et al., Microfluid Nanofluid.,20, 36,2016

[2]Miranda et al., J. Chem. Theory Comput., 14, 3113,2018

[3]Miranda et al., Scientific Rep.,6, 28128,2016

Designing phononic crystal with anticipated band structure through a deep learning based data-driven method

Zhanli Liu [1], Xiang Li [1], Shaowu Ning [1], Zhuo Zhuang [1]

[1] Applied Mechanics Lab., Dept. of Engineering Mechanics, School of Aerospace,

Tsinghua University, Beijing 100084 China

liuzhanli@tsinghua.edu.cn

Phononic crystal is a type of artificial heterogeneous material constituted by a periodic repetition of cells. This characteristic provides a possible solution to the accurate manipulation of acoustic and elastic waves. For this reason, phononic crystal is of application potentials in vibration and noise reduction, filtering, acoustic lens, acoustic imaging, and acoustic stealth, etc. It is thus of significance in the fields of information, communication and medical applications. To design phononic crystal with anticipated manipulation characteristic has become a research hotspot in recent years. However, how to accurately manipulate acoustic and mechanical wave is still a major challenge for existing designing approaches. Assisted by image-based finite element analysis and deep learning, a data-driven approach is proposed in this study for designing phononic crystals. An auto-encoder is trained to extract the topological features from sample images. Finite element analysis is employed to study the frequency bands of samples. A multi-layer perceptron is trained to establish the inherent relation between frequency bands and topological features. The trained models are ultimately employed to design phononic crystals with designated frequency bands. Not limited to this material, the proposed method could be further extended to design various structured mechanical materials with specific functionalities.

Stochastic Finite Element Analysis of U-Shaped RC Shear Wall with a Novel Random Field Modeling Strategy for Open Thin-Walled Structural Members

De-Cheng Feng[1], Yan-Ping Liang[2], Xiaodan Ren[3]

[1]School of Civil Engineering, Southeast University, dcfeng@seu.edu.cn

[2]School of Civil Engineering, Tongji University, 281455107@qq.com

[3]School of Civil Engineering, Tongji University, rxdtj@tongji.edu.cn

The inherent randomness of the material properties, with its coupling with the material nonlinear behaviors, often plays an important role in the analysis and design of structures. Furthermore, some quasi-brittle engineering materials, e.g., concrete, are often inhomogeneous, which means its material properties will vary from point to point within the domain of the structure. To comprehensively represent the mechanical behaviors of structures and elaborately reveal the corresponding damage/failure mechanisms, it is necessary to account for this spatially inhomogeneous effect. Generally, the Stochastic Finite Element Method (SFEM) is adopted to model inhomogeneous structures, in which the material properties are assigned as random fields. Up to date, several celebrated works have been proposed to represent the random field, e.g., spectral representation (SR) method, Karhunen-Loève expansion (KL) method, stochastic harmonic function (SHF) method, etc. However, most of the existing strategies are developed for the modeling of random fields spanning on the Euclidean space, e.g., a 2D plane space, while it remains a challenge for the definition of the random fields on manifolds and curved surfaces.

In the present work, a novel random field modeling strategy for open thin-walled structural members is developed. The manifold occupied by the open-thin walled structural member is mapped to the 2-D Euclidean space using the manifold learning methods, then the well-known random field representation methods can be directly employed. Theoretically, either SR, KL and SHF methods can be adopted. Nevertheless, considering the balance between numerical accuracy and computational efficiency, the SHF method is used herein due to the reduced number of basic random variables. The above mentioned strategy is then integrated with the softened damage-plasticity model, which can accurately reproduce the typical nonlinear behavior of quasi-brittle materials, to perform the stochastic finite element analysis. Moreover, the probability density

evolution method (PDEM) is also introduced to obtain the instantaneous probability density function of the structural responses through the results by SFEM. Finally, the proposed framework is applied to the analysis of U-shaped reinforced concrete shear walls, and the stochastic behaviors, e.g., bearing capacity, energy dissipation and damage evolution, are obtained and discussed.

Increased Modelling Demands by Moving from Resolved to Unresolved Simulation of Heterogeneous Reactive Systems

Bahram Haddadi[1], Christian Jordan[1], Michael Harasek [1]

[1]Technische Universität Wien, ICEBE

bahram.haddadi.sisakht@tuwien.ac.at

Catalysts can be used for speeding up reactions. For a certain catalytic reaction, the surface area of the catalyst available to the reactants plays an important role in the performance of the processes. Packed beds are a robust solution for increasing the surface area between fluid and solid because of their stable and economic operation. The catalytic reaction behavior in the packed can be investigated whether experimentally or using simulation approaches. Although experiments can provide valuable information about the system, they are time consuming and costly. On the other hand, verified simulation approaches can provide detailed information about the processes in a reasonable cost.

Among available simulation approaches, computational fluid dynamics (CFD) is a valuable tool for investigating mentioned heterogeneous systems, since it can provide time and space resolved information. The main reason that lagged CFD in this field behind compared to the other simulation methods is the very high computational overhead for simulating these systems in fully resolved mode – resolving the geometry of each particle. This drawback can be overcame by simulating packed beds using an unresolved approach. In the unresolved approach, particles are not resolved but models are used for describing their effect on the flow and reaction behavior. For choosing the appropriate models, the main point is the capability of the chosen models on representation of the local and global phenomena.

In this study, the effect of different void fraction (porosity) models on unresolved simulation of a catalytic reaction in a packed bed was investigated. Dehydrogenation of n-octyl alcohol (octanol) over Cu^0 catalyst was simulated in a packed bed with bed/particle ratio of approximately eight. The simulated bed was filled up to 200 mm, octanol vapor was entering from bottom of the bed, and the products were exiting from the top. As a reference, the resolved bed was simulated using the suggested reaction kinetics and equilibrium in the literature [1]. For simulating the bed using unresolved

approach two models were used for porosity changes along bed radius: constant porosity and a porosity profile using the de-Klerk correlation. The overall conversion at the end of the column is similar for all three beds. The radial distribution of the octanol concentration can be found in Figure 1. As it can be seen, using more accurate physical model (de-Klerk) represents the local phenomena better compared to the other global model.

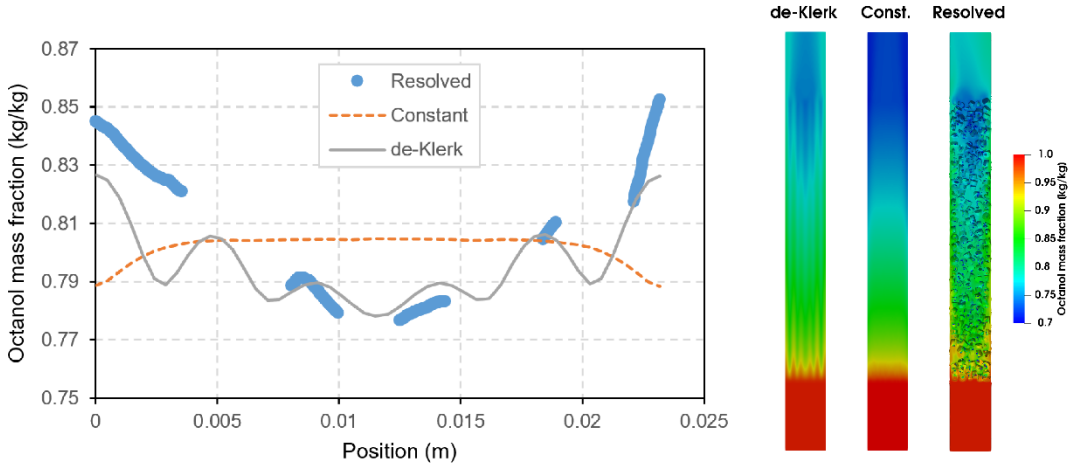


Figure 1. Octanol concentration at 0.1 m from bottom of a reactive catalytic packed bed. Resolved: catalytic particles surfaces are fully resolved – the local gaps in the graph show the particles positions, Constant: a constant radial porosity was used for unresolved modeling, de-Klerk: the radial porosity was modeled using de-Klerk correlation [2]

[1] M. E. Crivello, C. F. Pérez, S. N. Mendieta, S. G. Casuscelli, G. A. Eimer, V. R. El'\ias, and E. R. Herrero, "n-Octyl alcohol dehydrogenation over copper catalysts," *Catal. Today*, vol. 133, pp. 787–792, 2008.

[2] A. De Klerk, "Voidage variation in packed beds at small column to particle diameter ratio," *AIChE J.*, vol. 49, no. 8, pp. 2022–2029, 2003.

A Turbulence Based Sensitivity Study on Drag Prediction of the NASA Common Research Model Aircraft

Şule Öztürk [1], Berkay Pirlepeli[1], Mehmet Yılmaztürk[1] & Melike Nikbay[1]

[1]Istanbul Technical University

ozturksu15@itu.edu.tr, pirlepeli18@itu.edu.tr, yilmazturkm@itu.edu.tr, nikbay@itu.edu.tr

A great amount of effort has been spent several years to obtain the accurate numerical solution of flow over transonic commercial aircrafts and other aerospace industries by using the tools of Computational Fluid Dynamics (CFD). Estimation of the proper drag coefficient has been the most challenging with compared to the all other aerodynamic coefficients. There is a great deal of works to develop the CFD tools namely the geometry modeling, grid generation, numerical algorithms and turbulence modeling to get the proper and efficient solution of Reynolds-Averaged Navier-Stokes (RANS) equations for the flow field of complete aircraft configurations. One of the most important of these studies is the drag prediction workshops focused on the Common Research Model (CRM) Aircraft organized by National Aeronautics and Space Administration (NASA). [1]

The purpose of this study is to examine the structural and aerodynamic characteristics also the sensitivities of the turbulence model closure constants on the aerodynamic coefficients of NASA's CRM. For this purpose, Fluid Structure Interaction (FSI) and the CFD simulations will be performed on the Wing-Body-Tail (WBT) geometry using a commercial (FLUENT) software and an open source (SU2) software. Assuming the given reference flow conditions, the analyzes were carried out at different angle of attacks. The RANS equations were solved with Spalart-Allmaras(SA) and Menter's SST k-ω (SST) turbulence models. To verify the fidelity of simulations, the results will be compared with experimental and other study results. Finally, to determine the effect of SA and SST closure constants on the aerodynamic coefficients, a sensitivity study will be performed using Sobol indices and the optimal values for the turbulence model parameters will be determined. During studies all the necessary data and geometries are received from NASA. [2]

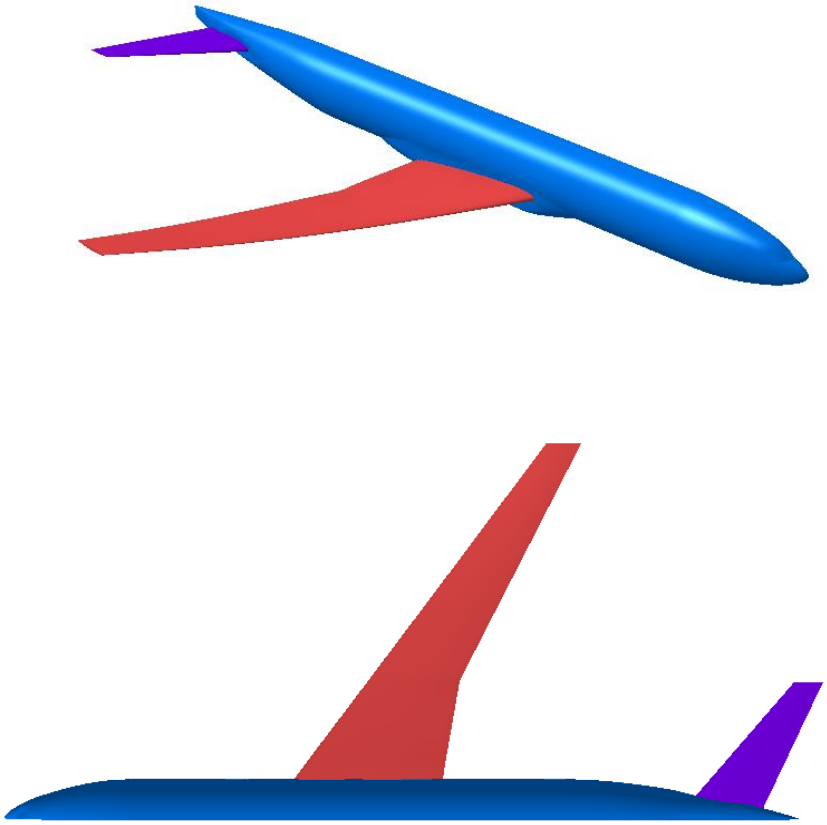


Figure 1 NASA CRM Aircraft WBT Geometries [2]

REFERENCES

[1] *6th AIAA CFD Drag Prediction Workshop* Retrieved April 14, 2019, from https://aiaa-dpw.larc.nasa.gov/

[2] *NASA Common Research Model* Retrieved April 14, 2019, from https://commonresearchmodel.larc.nasa.gov/2012/01/19/hello-world-2/

Approximation of frequency response functions with the multi-element generalised polynomial chaos method

Prem Ratan Mohan Ram [1], Ulrich Römer [1]

[1]Institut für Dynamik und Schwingungen, Technische Universität Braunschweig

p.mohan-ram@tu-bs.de

While designing or analyzing engineering systems, it is often the case that one is interested in analysing the effects of input uncertainties on response functions in the frequency domain. In cases where such a response is computationally expensive to compute, it becomes particularly necessary to compute a cheap surrogate model for uncertainty quantification purposes. It is also desired that such a surrogate is able to approximate the response accurately throughout the operating frequency range.

In many cases, while dealing with acoustic or electromagnetic systems for instance, this is quite challenging as it is common for these systems to exhibit sharp variations in their response for small changes in frequency. Lately two approaches, namely the Padé approximation technique and the polynomial chaos method are receiving increasing interest in this context. A general formulation of Padé-type approximations for multi-variate problems is still a work-in-progress [1]. The polynomial chaos method, on the other hand, requires a very high polynomial order to accurately approximate such response functions. Instead of using a high polynomial order on a global polynomial chaos expansion (GPCE) for the entire parameter domain, in [2], the multi-element generalized polynomial chaos expansion (MEGPCE) method has been proposed, which adaptively decomposes the domain of the random parameters into sub-domains, for each of which a local polynomial chaos expansion is computed. This allows using smaller elements at areas where the response varies sharply and larger elements elsewhere, thus performing a piecewise polynomial approximation.

In this work, we analyse the use of the MEGPCE to approximate frequency response functions which depend on random model parameters. Special emphasis is put on suitable error estimation techniques, which are required for adaptivity. In the original work [2] a variance-based criterion for adaptivity was proposed, which is easily computable in a polynomial chaos context. As pointed out in [3], using the relative

variance error as an indicator involves comparing this error against a free parameter, which lacks a physical meaning, to decide whether a particular element has to be further divided or not. In [3], this problem of fixing a free parameter is avoided by using the residual error, computed by using the approximated solution in the governing system of equations, to steer the MEGPCE algorithm. We additionally investigate the use of an adjoint error indicator [4] in the MEGPCE, which indicates the error in approximating the actual quantity of interest. Such an error indicator, being goal-oriented, promises quick convergence to the required quantity of interest.

We apply the MEGPCE to approximate frequency response functions of systems of the form

$$(-\omega^2 M + i\omega C + K)X = F \qquad (1)$$

, where the mass (M), damping (C) and stiffness matrix (K) may contain random input parameters. The behavior of several mechanical and electronic systems can be modelled with (1). We give several numerical examples and analyse the convergence of the MEGPCE method in approximating frequency response functions. Moreover, we assess and report on the efficiency of different error criteria mentioned above.

References:

[1] T. Chantrasmi, A. Doostan, G. Iaccarino, Padé–Legendre approximants for uncertainty analysis with discontinuous response surfaces, Journal of Computational Physics 228 (2009) 7159–7180

[2] X. Wan, G. E. Karniadakis, An adaptive multi-element generalized polynomial chaos method for stochastic differential equations, Journal of Computational Physics 209 (2005) 617–642

[3] B. Chouvion, E. Sarrouy, Development of error criteria for adaptive multi-element polynomial chaos approaches, Journal of Mechanical Systems and Signal Processing 66, DOI: 10.1016/j.ymssp.2015.05.007

[4] T. Butler, P. Constantine, T. Wildey, A posteriori error analysis of parameterized linear systems using spectral methods, SIAM J. Matrix Anal. Appl. 33 (2012) 195–209

Optimization of Control Parameters for an Electrified Vertical Take-off Landing Vehicle Using the Integral Squared Method

Ibrahim Cicek [1] and Prof. Dr. Melike Nikbay[2]

Istanbul Technical University

cicekib@itu.edu.tr

nikbay@itu.edu.tr

Electrified vertical take-off and landing (EVTOL) aircrafts are studied on contemporarily for their robust maneuvers and cost efficient flight operations. By mounting electric propulsion systems, EVTOLs are considered clean vehicle for next generation air transportation. To optimize flight performance of an EVTOL by minimizing power consumption and maintaining smooth maneuvers, the sought after values of control parameters are computed using the optimal control theory. System is to be modeled as closed loop linear control system with calibretable parameters. The aim is to tune control parameters sequentially by determining desired performance output resulting from the sequential inputs.

In this paper, a study on optimization of electrified vertical take-off landing aircraft control parameters is achieved by eliminating Integral Squared Errors - ISE method using the optimal control theory. Literally, error to be eliminated is discrepancy between target reference and actual state of flight maneuvers, when actuator inputs and systems response mismatch. In this case, the employed performance parameters are rise time, settling time and percentage overshoot of vehicle states over a specified time interval. These parameters are input for performance measure function which is objective function of the problem. System constraints are predefined for vehicle flight comfort and implemented into the Lagrange Multiplier Method for constrained non-linear optimization. Moreover, the method of eliminating steady state error is described by Parseval's Theorem for linear control systems.

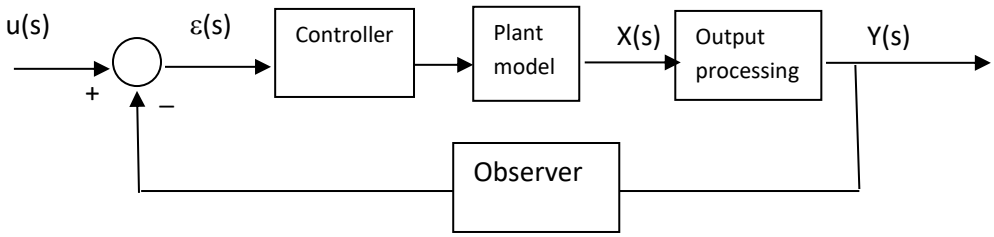


Fig1. Optimized system control scheme

The problem is modeled by mathematical representation of optimization probles as shown below with integral squared error measure J and predefined constraint C, eq(1) and eq(2). Parameters which related performance measure are are a, b, n ,m constants and calculation is done within time interval of [t=0, t_f] . Here t_f is arbitrary.

Minimize the defined performance index ;

$$J^* = \int_0^{t_f} \varepsilon(t)^2 dt$$

Subject to performance measure of;

$$C = \int_0^{t_f} a[X(t)^n \pm bY(t)^m]dt$$

Where C is constrained between limits of –k < C < +k.

References

[1] D.E. Kirk, *Optimal Control Theory An Introduction*, 1970, Prentice Hall, New Jersey.

[2] M. Nikowitz, *Advanced Hybrid and Electric Vehicles System Optimization and Vehicle Integration*, 2016, Springer, Vienna Austria.

[3] Y.S. Wang, *A System Level Approach to Optimal Controller Design for Large-Scale Distributed Systems, 2017*, California Institute of Technology.

[4] Y.L. Leong, *Optimal Controller Synthesis for Nonlinear Systems, 2017*, California Institute of Technology.

Assessment of the Size of the Representative Volume Element of Random Heterogeneous Materials

Paweł Hołobut [1]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences

pholob@ippt.pan.pl

One of the main concepts in micromechanics of materials and homogenization theory is the Representative Volume Element (RVE). There exist several imprecise definitions of the RVE, describing in qualitative terms a similar entity. The RVE is generally understood as a cubic volume of material which is macroscopically small, but simultaneously large enough to well represent the material's microstructural features in the statistical sense. In particular, the RVE's overall physical properties should be effective in the sense of being invariant with respect to choosing a different sample or further increasing the size of the cube. The RVE size depends on the physical property being considered (elastic or plastic properties, thermal conductivity, etc.), geometry of the microstructure (number of phases and their spatial arrangement), and the differences between the properties of individual phases [1]. The RVE is generally assumed to be large compared with the size of inhomogeneities; however, effective properties can sometimes be estimated using cubes of relatively small sizes [2].

In periodic materials, the RVE can be selected as the elementary periodic cell. In heterogeneous materials with random morphology, however, determination of the size of the RVE is not straightforward. Due to random spatial variations of the microstructure, two samples of the same random material may differ in their average response beyond an acceptable tolerance limit. This problem is frequently investigated using the notion of the Stochastic Volume Element (SVE) [3]. The SVE is a mesoscale volume element, whose size varies between the average size of inhomogeneities and the size of the RVE. The overall properties of the SVE, called apparent properties, are functionals over random fields describing the microstructure and may have significantly different values for different samples. As the size of the SVE increases, more and more inhomogeneities tend to be enclosed in the cube and the laws of large numbers cause that apparent properties tend to effective ones with increasing certainty. In this way, the SVE approaches the RVE.

The present work is devoted to probabilistic analysis of the size of the cube at which the transition from the SVE to the RVE can be assumed to occur. An attempt will be made to provide a precise, quantitative stochastic definition of the RVE, denoting an SVE of such dimensions that the probability of obtaining two samples with apparent properties differing by more than a given error threshold is sufficiently small. This is a slight modification and formalization of the approach proposed in [1]. Fundamental stochastic characteristics such as mean values and covariance matrices of apparent mechanical properties of SVEs will be presented for several example morphologies. Using the proposed definition of the RVE and the computed stochastic characteristics, approximate RVE sizes will be obtained and validated against results of numerical homogenization.

References

[1] T. Kanit, S. Forest, I. Galliet, V. Mounoury, D. Jeulin. *Determination of the size of the representative volume element for random composites: statistical and numerical approach*. International Journal of Solids and Structures, Vol. 40, pp. 3647–3679, 2003.

[2] A. El Moumen, T. Kanit, A. Imad, H. El Minor. *Effect of reinforcement shape on physical properties and representative volume element of particles-reinforced composites: Statistical and numerical approaches*. Mechanics of Materials, Vol. 83, pp. 1–16, 2015.

[3] M. Ostoja-Starzewski. *Material spatial randomness: From statistical to representative volume element*. Probabilistic Engineering Mechanics, Vol. 21, pp. 112–132, 2006.

Scaling procedure for the design of a validation experiment on an accidental gas release

Anna Chiara Uggenti[1], Alberto Moscatello[1], Gaetano Iuso[1], Domenic D'Ambrosio[1], Gioacchino Cafiero[1], Raffaella Gerboni[1], Andrea Carpignano[1]

[1]Politecnico di Torino, Corso Duca degli Abruzzi, 24, Torino, Italy

anna.uggenti@polito.it, alberto.moscatello@polito.it, gaetano.iuso@polito.it, domenic.dambrosio@polito.it, gioacchino.cafiero@polito.it, raffaella.gerboni@polito.it, andrea.carpignano@polito.it

Oil&Gas platforms are complex structures characterized by the presence of flammable and pressurized fluids and by a unique working environment, with limited spaces and congested presence of processing equipment. Risk assessment on these structures is mandatory according to international directives and it involves the evaluation of frequencies and consequences of possible accidental scenarios.

The Italian Ministry of Economic Development is supporting the SEADOG (Safety and Environmental Analysis Division for Oil&Gas) laboratory at Politecnico di Torino to develop research projects on Oil&Gas offshore safety. At SEADOG, we have developed an innovative CFD hybrid approach to simulate the consequences of accidental gas releases.

This approach simulates two separate and consequent steps that happen in an accidental gas jet release: the first one is the initial supersonic behavior modeled into a portion of the total platform domain; the second step is the following subsonic dispersion of the released gas into the total domain. The supersonic characteristics appear within the first tens of centimeters from the release point, where the compressibility effects drive the phenomena evolution. The subsonic dispersion domain may corresponds to entire platform (tens of meters), where the fluid can be treated as incompressible. The two steps are computationally evaluated and optimized separately, while the coupling follows.

A key boundary condition for the phenomenon simulation is the wind speed. This real scale speed has to be defined according with the typical velocity distribution of the atmospheric wind present in the location (Adriatic Sea) where the platform is positioned.

To validate this theoretical approach, a physical experiment is designed for the investigation in a wind tunnel of a scaled (1:10) mockup of a real platform will be equipped with a gas release supply line and a sensors' network.

While the mock up is scaled according to a geometric ratio, a finer assessment is needed to apply the correct scaling approach to define the reference speed in the wind tunnel and the mass flow release.

The scaling of the wind velocity has followed the scaling theory for wind tunnels, respecting the logarithmic evolution of the wind profile in proximity to the sea surface.

The scaling of the mass flow release is inspired by the approach proposed by Hall and Walker (1997) with some adjustments to fit our specific case.

In particular, a dimensionless group is chosen to link pressure release, nozzle diameter, scaling factor and gas properties: the dimensionless discharge momentum flux. Furthermore, this group contains information about both the real and the scaled wind velocity.

The approach proposed in this paper aims at scaling supersonic jet releases, maintaining their critical behavior for the test.

A selection of case studies will be tested in the experimental setup to be built by the end of year 2019 under the supervision of the SEADOG research team.

Reference

Hall D. J. and Walker S., "Scaling rules for reduced-scale field releases of hydrogen fluoride", Journal of Hazardous Materials, vol. 54, pp. 89-111 (1997)

A DFT study of single layer blue phosphorus and its implementation in a continuum model

Farzad Shirazian [1], Reza Ghaffari [2], Ming Hu [3], Roger A. Sauer [4]

[1,2,4] Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Templegraben 55, 52056 Aachen, Germany

[3] Department of Mechanical Engineering, University of South Carolina, 541 Main Street, Columbia, SC 29208, USA

[1] shirazian@aices.rwth-aachen.de

[2] ghaffari@aices.rwth-aachen.de

[3] hu@sc.edu

[4] sauer@aices.rwth-aachen.de

The mechanical properties of single layer blue phosphorus are studied using density functional theory (DFT). The simulations are carried out using the Quantum Espresso package [1]. An ultrasoft pseudopotential and the Perdew-Burke-Ernzerhof (PBE) exchange correlation functional are used in the DFT simulations. The considered unit cell is periodic and consists of two phosphorus atoms. In order to eliminate the interaction with replicates in the out-of-plane direction, a vacuum space has been considered in the unit cell.

First, the atomic structure of blue phosphorus is obtained. The lattice parameter is 3.28 Å, the thickness of the monolayer is 1.23 Å, and the length of the P-P bond is 2.26 Å. Then, an optimal set of virtual tests is designed to obtain the mechanical behavior of blue phosphorus. Two uniaxial stretches along the zigzag and armchair directions and one pure dilatation virtual test are chosen, and the strain energies and stresses are calculated for various strains. At each step, the strain is applied to the boundary of the unit cell and the atoms are relaxed while keeping the unit cell fixed.

The generated data are then used to calibrate a nonlinear, hyperelastic, and anisotropic continuum model that is then implemented in the curvilinear rotation-free finite shell element formulation of [2]. The employed framework has been previously used for the development of membrane and shell material models for graphene [3, 4, 5].

The model is then used to simulate the micro-indentation of single layer blue phosphorus as an example.

In order to validate the model and show its ability to capture anisotropic behavior of single layer blue phosphorus, the virtual uniaxial stretch test is conducted in other directions. The results are presented in Fig. (1). The continuum model shows good agreement with DFT calculations. More results are available in [6].

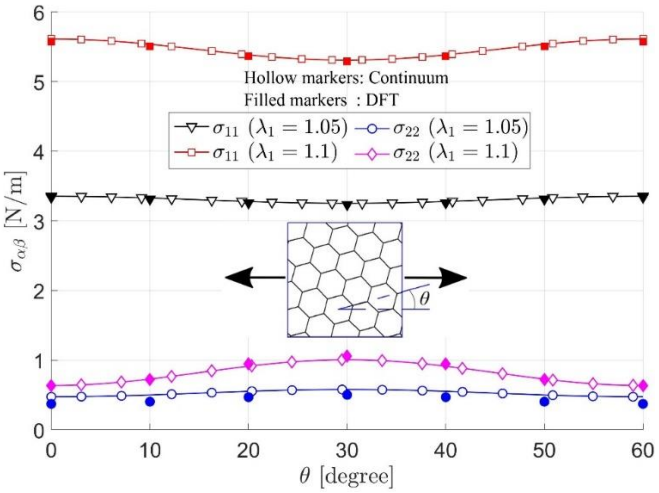


Figure 1: Comparison of the DFT and continuum results for stress σ_{11} and σ_{22} for a stretch in direction θ with respect to the armchair direction. The figure is taken from [6].

REFERENCES

[1] P. Giannozzi et. al. Quantum espresso: a modular and open-source software project for quantum simulations of materials. J. Phys. Condens. Matter, 21(39):395502, 2009.

[2] Thang X. Duong, Farshad Roohbakhshan, and Roger A. Sauer. A new rotation-free isogeometric thin shell formulation and a corresponding continuity constraint for patch boundaries. Comput. Methods in Appl. Mech. Eng., 316(Supplement C):43-83, 2017. Special Issue on Isogeometric Analysis: Progress and Challenges.

[3] Sandeep Kumar and David M. Parks. On the hyperelastic softening and elastic instabilities in graphene. Proc. Royal Soc. Lond. A: Math. Phys. Eng. Sci., 471(2173), 2014. DOI: 10.1098/rspa.2014.0567.

[4] Reza Ghaffari, Thang X. Duong, and Roger A. Sauer. A new shell formulation for graphene structures based on existing ab-initio data. Int. J. Solids Struct., 135:37-60, 2018.

[5] Reza Ghaffari and Roger A. Sauer. A new efficient hyperelastic finite element model for graphene and its application to carbon nanotubes and nanocones. Finite Elem. Anal. Des., 146:42-61, 2018.

[6] Reza Ghaffari, Farzad Shirazian, Ming Hu, and Roger A. Sauer. A nonlinear hyperelasticity model for single layer blue phosphorus based on ab-initio calculations. arXiv e-prints, page arXiv:1902.05128, Feb 2019.

A Fully Second-Order Homogenisation Model for the Analysis of Multi-Phase Materials at Finite Strains

Igor A. Rodrigues Lopes [1], Francisco M. Andrade Pires [2]

[1,2] Faculty of Engineering of the University of Porto, INEGI

[1] ilopes@fe.up.pt, [2] fpires@fe.up.pt

Multi-scale analyses are of utmost importance in order to understand the micro-scale mechanisms that influence the macroscopic material behaviour. Materials which are heterogeneous at a certain spatial scale may be modelled by a Representative Volume Element (RVE), where phenomena arising at the micro-scale due to a macro-scale loading may be analysed in detail, accounting for the effect of material heterogeneities.

Second-order homogenisation-based multi-scale models where the macro-scale is modelled as a second-order continuum, while the micro-scale is described by the classical first-order continuum mechanics [1,2,3], enable the modelling of moderately high strain gradients at the macro-scale and allow the analysis of deformation modes like bending or torsion at the micro-scale. In addition, the homogenised response is influenced by the RVE length, that acts as a length-scale parameter in the macro-scale constitutive response. Nevertheless, this kind of models is not able to capture size effects due to the length of the micro-constituents.

In the present contribution, a fully second-order homogenisation model, where the material behaviour is modelled with a second-order continuum at both scales, is formulated. Due to the characteristic length introduced at the micro-scale through the second-order constitutive equations, the influence of the constituents' size is included in the model. The numerical solution of the resulting micro-macro coupled problem is described in detail with mixed finite elements. Illustrative examples are employed to show the capabilities of the presented model to describe distinct aspects of the material behaviour at both scales.

REFERENCES

1. V.G. Kouznetsova, M.G.D. Geers and W.A.M. Brekelmans, Multi-scale constitutive modelling of heterogeneous materials with a gradient-enhanced computational homogenization scheme. *Int. J. Numer. Meth. Eng.*, Vol. **54**, pp. 1235-1260, 2002.

2. D.J. Luscher, D.L. McDowell and C.A. Bronkhorst, A second gradient theoretical framework for hierarchical multiscale modeling of materials. *Int. J. Plast.*, Vol. **26**, pp. 1248-1275, 2010.
3. P.J. Blanco, P.J. Sánchez, E.A. de Souza Neto and R.A. Feijóo, The method of multiscale virtual power for the derivation of a second order mechanical model. *Mechanics of Materials*, Vol. **99**, pp. 53–67, 2016.

Ductile failure analysis in metallic materials through computational homogenisation

R. P. Cardoso Coelho [1], D. de Bortoli [1], R. Pinto Carvalho [1], F. M. Andrade Pires [1]

[1]Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI), Faculty of Engineering, University of Porto

{ruicoelho,ddbortoli,rcarvalho,fpires}@fe.up.pt

The ductile failure of metals at low homologous temperatures is largely determined by the nucleation, growth and coalescence of microstructural voids. These phenomena are strongly dependent on the stress state, specifically on parameters such as triaxiality and Lode angle. High triaxiality stress states tend to increase the void size, whereas lower triaxialities distort them significantly. The Lode angle has a smaller but still noticeable effect on ductile failure. Over the last years, the modeling of heterogeneous materials by an interchange of information between the macro and micro scales has received increasing attention, especially by the analysis of microscopic Representative Volume Elements (RVEs) and the homogenization of its response to obtaining its macroscopic counterpart[1,2].

The main purpose of this contribution is to investigate the influence of factors such as loading path, material properties and void geometry on the overall macroscopic response. Using the finite element method, several RVEs containing voids are analyzed, subjected to different boundary conditions, with both isotropic (von Mises) and anisotropic (mono- and polycrystalline FCC and BCC slip) matrix material models. A stress driven homogenization approach is used, allowing for strict control over both triaxiality and Lode angle. Furthermore, parametric studies are conducted in terms of the void geometry, porosity, triaxiality and Lode angle. The results obtained are then used to critically assess analytical models available in the literature (e.g. [3]).

[1] Luo T., Gao X., 2018. On the prediction of ductile fracture by void coalescence and strain localization. Journal of the Mechanics and Physics of Solids 113, 82-104.

[2] Zhou J., Gao X., Hayden M., Joyce J. A., 2012. Modeling the ductile fracture behavior of an aluminum alloy 5083-H116 including the residual stress effect. Engineering Fracture Mechanics 85, 103-116.

[3] Mbiakop A., Constantinescu A., Danas K., 2015. An analytical model for porous single crystals with ellipsoidal voids. Journal of the Mechanics and Physics of Solids 84, 436-467.

Computational Aspects on the Constitutive Modelling of Multiphase Alloys

M. Vieira de Carvalho[1], D. de Bortoli[2] and F.A Andrade Pires[3]

[1]FEUP, University of Porto, mvcarvalho@fe.up.pt

[2]INEGI, University of Porto, ddbortoli@fe.up.pt

[3]FEUP, University of Porto, fpires@fe.up.pt

Multiphase alloys, such as TRIP (transformation induced plasticity) and dual-phase steels, enjoy considerable technological importance, due to their increased strain hardening capacity, i.e. the combination of high yield strength and elongation at failure. However, the complex microstructural phenomena involved – such as plastic slip and martensitic phase transformations – pose a number of computational challenges.

In this work, several aspects of the computational treatment of constitutive models for such materials are explored, using a crystal plasticity-like model accounting for both plastic slip and martensitic transformations [1]. The model's evolution equations are solved using a fully implicit algorithm that employs a volume-preserving exponential map integrator [2], which is critical for the accurate modelling of incompressible plastic deformations. A rate-dependent regularisation [3] to the original equations is pursued to circumvent a number of difficulties appearing in the elastoplastic formulation, including: non-smooth yield functions, non-unique solutions and, in particular, the formulation of robust algorithm for determining the incremental set of active slip and transformation systems.

The ensuing numerical difficulties – primarily due to the well-documented equation stiffness in the rate-independent limit of vanishing viscosity parameters – are addressed with a number of algorithmic strategies. These include a consistent sub-stepping scheme at the stress update level, the iterative variation of rate-sensitivity material parameters, a procedure to remove the rate dependence of the regularised viscoplastic formulation, and the integration of the critical resolved stress evolution using a generalised mid-point rule.

The formulation presented is exactly linearised, at both the local (stress update) and global level, so that quadratic rates of assymptotic convergence are possible when using a Newton-Raphson scheme in a finite element solution. The impact of the strategies adopted in the overall efficiency and accuracy of the numerical solution to the constitutive equations is assessed in a number of examples, including the macroscopic response of polycrystalline RVEs.

References:

[1] D. de Bortoli, F. Adziman, E.A. de Souza Neto, F.M. Andrade Pires, "Constitutive modelling of mechanically induced martensitic transformations: Prediction of transformation surfaces", Engineering Computations, 35, 772–799 (2018).

[2] 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).

[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).

A Finite-Strain Elasto-Viscoplastic Model for Rubber Toughened Glassy Polymers: Formulation and Validation

Bernardo P. Ferreira[1], S. M. Mirkhalaf [2], Francisco M. Andrade Pires[1]

[1]Department of Mechanical Engineering, Faculty of Engineering, University of Porto,

bpferreira@fe.up.pt, fpires@fe.up.pt

[2]Chalmers University of Technology, University of Gothenburg,

m.mirkhalaf@gmail.com

Over recent years, the modeling of heterogenous multi-phase materials has been a topic of extensive research by the scientific community. Among other approaches, computational homogenization-based multiscale 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.

A considerable effort has been made by the scientific community to develop constitutive models that are able to accurately describe the deformation behaviour of polymeric based materials. Concerning their fracture thoughness, it is well known that glassy polymers show brittle behaviour, particulary under specific conditions such as low temperatures and high strain rates. One important and well-known technique to improve their fracture toughness is termed rubber toughnening, which consists in dispersing rubbery particles in the polymeric matrix in order to hinder the propagation of microfractures. Associated with these rubbery particles is the phenomenon of internal cavitation, meaning that they will behave as voids during the deformation of the rubber toughened polymer.

Polimeric based materials have been studied and modeled at different scales in order to capture their complex deformation behaviour. This model fully couples the finite strain elasto-viscoplastic constitutive model proposed by Mirkhalaf et al. [1] with the yield surface of the well-known micromechanical void growth model proposed by Gurson [2]. In the first place, several parametric studies are conducted in order to verify if the model is able to capture the main features of the rubber toughened glassy polymers characteristic behaviour. The predictive ability of the continuum model is then assessed by comparison with the homogenized response of a voided representative volume element, obtained with a first order homogenization-based multiscale model [3].

[1] Mirkhalaf, S. M., Pires, F. M. A., and Simoes, R. (2016). An elasto-viscoplastic constitutive model for polymers at finite strains: Formulation and computational aspects. Computers and Structures, 166:60–74.

[2] 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.

[3] Reis, F.J.P. & Andrade Pires, F.M. (2013). An Adaptative Sub-incremental Strategy for the Solution of Homogenization-based Multi-scale Problems, Computer Methods in Applied Mechanics and Engineering, Vol. 257, pp. 164– 182.

PGD based domain decomposition method applied to parameterized seismic models

Prattya Datta[1,2], David Modesto[1,2], Josep De La Puente[2] and José María Cela Espín[1,2]

[1]Universitat Politècnica de Catalunya

[2]Barcelona Supercomputing Center

prattya.datta@bsc.es

One of the key steps to generate a seismic image is to solve the parametric Helmholtz equation iteratively. A typical Helmholtz model is solved in a spatial dimension of 10-15 kms and high frequencies. Solving such a large scale model for different parameters requires extensive computations and hence an extremely resource intensive process. The proper generalized decomposition (PGD) technique can be used to accelerate this iterative process by means of real-time evaluations of a surrogate Helmholtz model. Unfortunately, standard PGD methods applied to wave problems are extremely penalized if the global parametric domain imposes large variations along the frequency dimension. More precisely, PGD convergence to a global solution usually fails even when optimized algorithms for non-hermitian problems are applied. This can preclude their application when realistic geophysical models are of concern.

In order to circumvent this issue, a first approach to combine domain decomposition (DDM) and PGD methods is presented for 2D spatial Helmholtz models. This strategy computes local surrogate models that retain the PGD convergence in spatially-decomposed domains, whereas the global convergence of the solution remains guaranteed by the choice of a proper spatial DDM strategy. In particular, the DDM transmission conditions on the boundaries of the sub-domains in the PGD model are defined by overlapped perfectly matched layers (PML). Overlapping PML transmission conditions in full order simulations have shown better global iterative convergences in the residual update, and also better endurance against dependencies on the number of selected sub-domains. Each sub-domain is solved in the reduced order space using the transmission conditions of PML. The global surrogate model is finally built by adding the spatial contribution of all the sub-domains. This process can be ensembled either in serial or parallel approach if HPC resources are available.

Fully coupled multi-scale finite element analysis of TRIP-assisted multi-phase alloys

D. de Bortoli[1,2], M. Vieira de Carvalho[1], I.A. Rodrigues Lopes[1], F.M. Andrade Pires[1]

[1] Computational Multi-Scale Modelling of Solids and Structures Research Group (CM2S), University of Porto, Porto, Portugal

[2] Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI), University of Porto, Porto, Portugal

{ddbortoli, mvcarvalho, ilopes, fpires}@fe.up.pt

With the ever-increasing demand for materials with improved performance, alloys such as advanced high-strength steels (AHSS) enjoy particular technological importance. This is due to their unusually favourable mechanical properties, such as a combination of both high strength and good ductility. To achieve that, these alloys exploit complex micro-structural phenomena, such as the *transformation-induced plasticity* (TRIP) effect, where mechanically induced phase transformations lead to increased overall strain hardening capability. From a modelling perspective, this interplay of deformation mechanisms across multiple phases and length scales is challenging. Capturing the complex material behaviour requires microstructure-aware models capable of reproducing fine-scale crystalline features. In this context, multi-scale models fit naturally, given their ability to both capture fine-scale crystalline features and relate them to the macroscopic, engineering scale.

Based on a recently proposed constitutive model for mechanically-induced phase transformations [1], a unified crystal-plasticity framework is used in this work to model the simultaneous evolution of crystallographic slip and martensite formation in metallic alloys. The constitutive model for mechanically induced phase transformations is based on a classical energy-based criterion for the martensite onset [2], generalised to multi-axial stress states and finite strains. The well-established Phenomenological Theory of Martensite Crystallography [3] is used to derive lattice-scale data on crystallographic transformation systems, which is used by the continuum, grain-scale model. Austenitic slip is modelled using a classical multi-surface crystal plasticity model, and the effects of anisotropic cubic elasticity are also taken into account.

Fully coupled, full-field two-scale finite element analyses (FE^2) are used to reproduce a series of structural experimental results for materials such as austenitic stainless steels and multi-phase TRIP steels, under a wide variety of loading conditions. The constitutive model is calibrated from micro-scale experiments performed on individual phases of TRIP steels. RVE size effects in such alloys are also investigated using a second-order homogenisation scheme. Results show that the proposed framework captures the experimentally observed material behaviour, such as the role of martensitic transformations in the overall mechanical response, highlighting the promise of the multi-scale approach in the modelling and design of advanced materials.

References

[1] D. de Bortoli, F. Adziman, E.A. de Souza Neto, F.M. Andrade Pires, "Constitutive modelling of mechanically induced martensitic transformations: Prediction of transformation surfaces", Engineering Computations, 35, 772–799 (2018).

[2] J.R. Patel, M. Cohen, “Criterion for the action of applied stress in the martensitic transformation”, Acta Metallurgica, 1 (5), 531–538 (1953).

[3] M.S. Wechsler, D.S. Lieberman, T.A. Read, “On the theory of the formation of martensite”, Transactions of AIME, 197, 1503–1515 (1953).

Computational methods for hybrid multiscale modelling in immunology

Dmitry Grebennikov [1,2], Gennady Bocharov [2]

[1]Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia

[2]Institute of Numerical Mathematics of the Russian Academy of Sciences, Moscow, Russia

dmitry.ew@gmail.com, bocharov@m.inm.ras.ru

The immune system is regulated by multiple processes at the genetic, cellular, tissue, organ and the whole organism scales. Therefore, its resulting complexity should be analyzed with hybrid multi-scale models. Virus-host interactions are widely modelled with ODE systems, and interacting components are treated as continuous variables. This approximation is correct only when the numbers of all variables are large enough, whereas the numbers of virions and infected cells are typically small at the initial stage of infection. To efficiently account for their discrete stochastic nature at the early stage, we developed an algorithm for hybrid modelling which utilizes the deterministic representation at the later stages [1].

We present a multiscale hybrid modelling approach which extends the initial model developed for analysis of HIV infection [2]. The multiscale model incorporates the spatio-temporal dynamics of immune cells, viruses and cytokines in lymphoid tissue and couples it with the virus- and cell population dynamics in blood. The locomotion of immune cells is governed by the force-based particle model which accounts for intercellular interactions, cellular intrinsic motility and viscous dissipation. The extracellular dynamics of cytokines is modelled with reaction-diffusion equations. Intracellular HIV replication and molecular regulation is described with ODE systems, and is coupled to the extracellular cytokine fields. Cell fate determining decisions depend on the concentrations of intracellular factors. The model is used to predict the requirements for the containment of HIV infection in local environments of lymphoid tissue. The research is funded by the Russian Science Foundation (grant 18-11-00171).

1. Sazonov I, Grebennikov D, Kelbert M, Bocharov G. *MMNP* (2017) **12**:63–77.

2. Bocharov G, Volpert V, Ludewig B, Meyerhans A. *Springer*, 2018, 221–242.

Multiscale stochastic simulations using a MFH model constructed from full-field SVE realizations

Juan Manuel Calleja Vázquez [1 2], Ling Wu [1], Van-Dung Nguyen [1], Ludovic Noels [1]

[1]Université de Liège

[2]jmcalleja@uliege.be

Nowadays experimental testing of composite materials represents a big challenge for companies, as a large number of tests are necessary to fully characterize a material. Virtual testing represents one of the best options for reducing dramatically these costs in the near future.

In order to make virtual testing become a real alternative for industry when characterizing the performance of a material, it is important not only to have a good representation of its deterministic behaviour, but to take into account all the stochastic non-determinisms that can be present in it: for example geometry variations in the microstructure due to the diposition of the fibers.

In this paper, an inverse Mean-Field Homogenization (MFH) model of a UD composite material used in industry is built from the homogenized stochastic behavior obtained by performing full-field simulations of Stochastic Volume Element (SVE).

As a first step, a micro-mechanical model of reinforced polymer failure with length scale effects is used to simulate the results obtained in tensile tests at constant speed rate of the epoxy used for the construction of the UD material. To this purpose, the complex polymer behavior is represented by a hyperelastic viscoelastic-viscoplastic constitutive model enhanced by a multi-mechanism nonlocal damage model (1). This law is composed of three components: hardening, saturation and failure laws. The characterization of the numerical parameters of the epoxy are obtained by simulating the experimental tensile test and matching the experimental energy release rate (G_c) of the material as developed in (2).

Once the micro-mechanical model of the epoxy is characterized, multiple full-field simulations of composite Stochastic Volume Element (SVE) realizations are performed to characterize the homogenized stochastic behavior of the composite,

information that will be used to build a MFH model as developed in (3). Once this model is constructed, efficient macro scale simulations of a ply failure taking into account geometrical variabilities of the microstructure are possible, bringing the industry closer to a possible future virtual testing of composite materials.

Bibliography

1. *A large strain hyperelastic viscoelastic-viscoplastic-damage constitutive model based on a multi-mechanism non-local damage continuum for amorphous glassy polymers.* **Nguyen, Van-Dung, et al.** 2016, International Journal of Solids and Structures, pp. 192 - 216.

2. *A micro-mechanical model of reinforced polymer failure with length scale effects and predictive capabilities. Validation on carbon fiber reinforced high-crosslinked RTM6 epoxy resin.* **Nguyen, Van-Dung, Wu, Ling and Noels, Ludovic.** 2019, Mechanics of Materials, pp. 193 - 213.

3. *An inverse micro-mechanical analysis toward the stochastic homogenization of nonlinear random composites.* **Wu, Ling, et al.** 2019, Computer Methods in Applied Mechanics and Engineering, pp. 97 - 138.

Simulation of adhesive squeeze flow using smoothed particle hydrodynamics

Lorraine A. Silva[1], Christine Espinosa[1], Lucas F.M. da Silva[2], Eric Paroissien[1], Frédéric Lachaud[1]

[1] Institut Clément Ader (ICA), Université de Toulouse, ISAE-SUPAERO, INSA, IMT MINES ALBI, UTIII, CNRS, 3 Rue Caroline Aigle, 31400 Toulouse, FranceInstitut Clément Ader (ICA)

[2] Department of Mechanical Engineering, University of Porto, 4200-465, Portugal

lorraine.silva@isae-supaero.fr; christine.espinosa@isae-supaero.fr; lucas@fe.up.pt; eric.paroissien@isae-supaero.fr; frederic.lachaud@isae-supaero.fr

In the last few years, so important than an optimized assembly is the Design for Disassembly or Demise (D4D). This conception has been implemented in many industries, for example, in the automobile with the recycling, recovery and reuse of End-of-Life Vehicles (ELVs) [1] and in the aerospace with the processing of the remaining materials for future aircrafts or other industrial applications [2]. Besides, even with the significant progress in that field there are some still recycling challenges, as examples, composite materials and polymers.

Among the many procedures for disassembling materials presented in the literature, the technique using Thermally Expandable Particles (TEP) developed by the FEUP is attractive due to its large potential application field [3]. The process of assembly can be divided into four steps: preparation, application, approach and curing. During the approach, the initial spot of adhesive is squeezed between the substrates. Depending on its compressibility, viscosity and on the roughness of the substrates, the final form of the adhesive will take and keep the shape of the mold, or even bleed in the free space between the substrates [4]. In the first case the thickness and even the particle distribution will be approximately uniform in the squeezed zone while they will not, may be, in the second case.

In this work we are interested in the simulation of the approach to predicting the final form of the adhesive using the smoothed particle hydrodynamics (SPH). The SPH is a meshfree method proposed by Gingold and Monaghan in 1964 [5] which has been the purpose of a lot of enhancements and represents today an elegant alternative solution for numerical simulations of fluids [6]. Simulating free surface movements or possible separation or mixture of different fluids is indeed very easy because the SPH

method is a mesh free technique that computes interactions between particles in a local neighborhood at chosen interval during deformation of the material.

The knowledge of the approach process allows addressing the squeeze flow problem in order to optimize the adhesive final distribution and the TEPs distribution and in the future the disassembly optimization.

[1] LU, Y., BROUGHTON, J., & WINFIELD, P. (2014). A review of innovations in disbonding techniques for repair and recycling of automotive vehicles. International Journal of Adhesion and Adhesives, 50, 119-127. https://doi.org/10.1016/j.ijadhadh.2014.01.021

[2] SABAGHI, M., CAI, Y., MASCLE, C., & BAPTISTE, P. (2016). Towards a sustainable disassembly/dismantling in aerospace industry. Procedia CIRP, 40, 156-161. https://doi.org/10.1016/j.procir.2016.01.088

[3] BANEA, M. D., DA SILVA, L. F., CARBAS, R. J. C., & DE BARROS, S. (2017). Debonding on command of multi-material adhesive joints. The Journal of Adhesion, 93(10), 756-770. https://doi.org/10.1080/00218464.2016.1199963

[4] ENGMANN Jan, SERVAIS Colin, BURBIDGE Adam S. (2005). Squeeze flow theory and applications to rheometry: A review. Journal of Non-Newtonian Fluid Mechanics, 132(1-3), 1-27. https://doi.org/10.1016/j.jnnfm.2005.08.007

[5] GINGOLD, R. A., & MONAGHAN, J. J. (1977). Smoothed particle hydrodynamics: theory and application to non-spherical stars. Monthly notices of the royal astronomical society, 181(3), 375-389. https://doi.org/10.1093/mnras/181.3.375

[6] LIU, G. R. & LIU, M. B. (Ed.). (2003). Smoothed particle hydrodynamics: a meshfree particle method. World Scientific. https://doi.org/10.1142/5340

A Thermo-Mechanically Coupled Cutting Simulation of Ti-6Al-4V Using Advanced Meshless Methods

M. Afrasiabi[1,2], M. Roethlin[1], H. Klippel[1,] K. Wegener[1]

[1] *ETH Zurich, Institute of Machine Tools & Manufacturing (IWF)*
[2] *ETH Zurich, Chair of Structural Mechanics & Monitoring at IBK*

Correspondence to: afrasiabi@ethz.ch

Metal cutting is an operation by which a layer of unwanted material from a given workpiece is removed. It remains one of the most important processes in today's manufacturing science and technology. Merchant [1] claimed in 1998 that up to 15% of the added production value of developed countries is associated with metal cutting operations. Hence, understanding such a process and optimization thereof plays an indispensable role in the advancement of new technologies and developments.

Despite their valuable insights into a better understanding of the mechanism, experimental studies do not suffice as adept tools for analyzing due to many reasons. The process is strictly dominated by large deformations and gradients, new surface generation, and extremely high strain rates, to name a few. On the other hand, the analytical solution to most of these operations does not exist, or in the best case scenario, is far from trivial. This investigation leaves the researchers with the simulation of the process.

Finite Element Method (FEM) has already established itself as the most popular choice for the simulation of metal cutting. However, it is nearly impossible nowadays to find a robust FEM solver that does not rely on adaptive remeshing procedures. Excellent accounts in this regard can be found in [2] and [3]. To release this cumbersome, and computationally expensive, procedure, a completely different approach can be considered which enables the spatial discretization using some Lagrangian points, called particles. The essential characteristics of the meshfree particle methods are that there is no need for a highly structured mesh as required in FEM. The most widely-used meshfree method to date is perhaps the Smoothed Particle Hydrodynamics (SPH) which was simultaneously introduced by Lucy [4] and Gingold et al. [5] in the late 70s.

In this work, a particle-based framework is developed to model a 2D orthogonal cutting of Ti-6Al-4V. To this end, a set of stabilization terms in addition to some corrective schemes are employed in an updated Lagrangian frame. Together with the stabilized SPH algorithm for the mechanical solver, a Particle Strength Exchange (PSE) method [6,7] is used for the heat conduction and thermal modeling. This choice is made based upon a great accuracy-performance trade-off that PSE offers in the discretization of higher-order derivatives, e.g., the Laplacian operator in the heat equation.

Yet another contribution of the present work lies in the adoption of a modified Johnson-Cook flow stress model, suggested by Sima et al. [8]. Motivated by the experimental and numerical results presented by the authors of [8], this constitutive model is herein chosen to capture the strain softening effect in the machining of titanium alloys. As illustrated in Figure 1, the proposed meshless solver is perfectly capable of representing the adiabatic shear bands and chip formation even in relatively low-resolutions. The results obtained from the meshless simulation stays in a good agreement with the available FEM and experimental data.

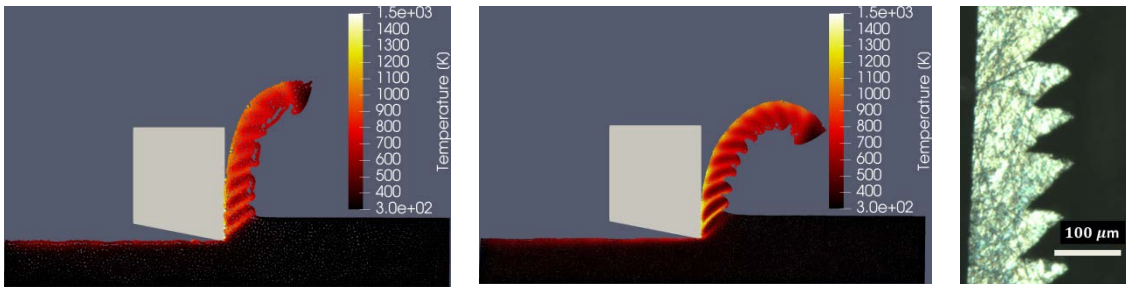


Figure 1. Temperature distribution and chip formation using the present method in low (left) and medium resolutions (middle). The chip shape (right) in experiment by [8].

Selected references

[1] M. Merchant, “An interpretive look at 20th century research on modeling of machining,” Machining Sc & Tech., 1998.
[2] P. Arrazola et al., “Recent advances in modelling of metal machining processes,” CIRP Annals-Manf., 2013.
[3] T. Marusich et al., “Modelling and simulation of high-speed machining,” IJNME, 1995.
[4] L. B. Lucy, “A numerical approach to the testing of the fission hypothesis,” The astronomical journal, 1977.
[5] R. A. Gingold and J. J. Monaghan, “Smoothed particle hydrodynamics: theory and application to nonspherical stars,” Monthly notices of the royal astronomical society, vol. 181, no. 3, pp. 375–389, 1977.
[6] S. Mas-Gallic and P. Raviart, “Particle approximation of convection-diffusion problems,” *Report of Univ de Paris*, 1986.
[7] J. D. Eldredge, et al., “A general deterministic treatment of derivatives in particle methods,” *JCP*, 2002.
[8] M. Sima and T. Özel, “Modified material constitutive models for serrated chip formation simulations and experimental validation in machining of titanium alloy ti–6al–4v,” *International Journal of Machine Tools and Manufacture*, 2010.

Multiphysics Simulation of Laser Metal Deposition Manufacturing Process Using a Meshless Method

Boussad Abbès [1], Fazilay Abbès [1], Tahar Anedaf [1], Yuming Li [1]

[1]GRESPI, University of Reims Champagne-Ardenne

boussad.abbes@univ-reims.fr, fazilay.abbes@univ-reims.fr, tahar.anedaf@etudiant.univ-reims.fr, yuming.li@univ-reims.fr

Laser Metal Deposition (LMD) is one the additive laser manufacturing technologies for obtaining complex metallic shapes and tools by adding lased material powder on a substrate. Furthermore, it has found an important application niche in the coating or repair of high value components as well as components that have undergone significant wear. It is used for example to repair turbine blades for the aerospace industry, drill pipes for offshore industry, injection molding tools for the automotive industry among others. To control the manufacturing process and the influence of the operating parameters on the final characteristics of the fabricated parts, it is important to understand the complex mechanisms involved in their manufacturing. Therefore, computational simulation has an important role to play in addressing these challenges.

This paper presents a three dimensional multi-physics models to describe the physical mechanism of heat transfer, melting and solidification that take place during the LMD process. The simulated transient temperature profile, the geometrical features of the generated structures and thermal cycles are presented. The results obtained from the model based on the meshless Finite Pointset Method (FPM), which is a variant of the Smooth Particle Hydrodynamics (SPH) method, provide the basis for the selection of the process parameters in additive manufacturing.

Micromechanical Modeling and Estimation of Elastic Properties of Pure MXene ($Ti_3C_2T_x$) Films

Krzysztof Grabowski [1] Shreyas Srivatsa [2] Tadeusz Uhl [3]

[1,2,3] AGH University of Science and Technology, Krakow, Poland

kgrabow@agh.edu.pl

MXenes are 2-dimensional (2D) materials made of metal carbides or metal nitrides. They have found a wide range of applications because of its hydrophilic and metallic behavior due to its surface termination and transition metal atoms, respectively. MXenes, particularly Titanium Carbide (Ti_3C_2) with surface termination (T_x) ($Ti_3C_2T_x$), have been used to fabricate pure MXene films and MXene/PVA nanocomposite. The MXene ($Ti_3C_2T_x$) monolayer (flake) elastic properties and Young's modulus (in the range of 300-360 GPa) are reported in the literature from Molecular Dynamics results and nanoindentation tests. The MXenes flakes stack up, one on top of the other, to form pure MXene film. Though limited experimental results are available in the literature, both analytical and numerical models for the pure MXene film are to be developed for the purpose of mechanical property estimation.

The focus of the paper is on the micromechanical modeling of pure MXenes ($Ti_3C_2T_x$) and estimation of the elastic properties of the MXene stack. MXenes are modeled as thin plate structures in microscale as the lateral dimensions of the MXene flakes are in the range of 2-10 microns and the thickness is in the range of 1-2 nanometers.

First, an analytical method is used to perform investigations. Classical Laminate Plate Theory (CLPT) which is based on Kirchhoff's plate theory assumptions, is used to model the MXene stack which forms the pure MXene film. The stiffness matrix and Young's modulus of the MXene stack are estimated based on this analytical model. The bonding between one MXene flake to another plays a crucial role in the estimation of Young's modulus of pure MXene stack. Therefore, in this paper, the bonding layer between the MXene flakes is considered and is termed as an interface layer. The Young's modulus of this interface layer is estimated based on the overall MXene stack Young's modulus reported in the literature on MXene films. The effect of the geometric and

material properties of the interface layer on the overall pure MXene stack elastic properties is studied.

Second, pure MXene is subjected to numerical modeling and analysis using Finite Element Method. They are modeled as a single layer, double layer and stack of MXenes with interface between them. The models are subjected to tensile loads in-plane with the MXene. The results of the simulations are reported in this paper. The results indicate a future work that the interface layer properties and behavior between MXene flakes need detailed modeling in the sub-micron scale using Molecular Dynamics which can improve the micromechanical model estimation.

Computational study of deformation mechanisms in hcp metal: Application to pure zinc

Fazilay Abbès [1], Nhan P. T. Nguyen [1, 2], Jean-Sébastien Lecomte [3], Christophe Schuman [3], Boussad Abbès [1]

[1]GRESPI, University of Reims Champagne-Ardenne,
[2]University of Danang, [3]LEM3, University of Lorraine

fazilay.abbes@univ-reims.fr, pham-the-nhan.nguyen@etudiant.univ-reims.fr, jean-sebastien.lecomte@univ-lorraine.fr, christophe.schuman@univ-lorraine.fr, boussad.abbes@univ-reims.fr

Zinc metal is well-known for its high corrosion resistance in most environments, which accounts for its successful use as a protective coating on a variety of products and in many exposure conditions, especially in automotive and building applications. Zinc has a hexagonal close-packed (hcp) crystalline structure. Compared to other hcp metals like titanium or magnesium, zinc exhibits a strong anisotropic behavior. Due to the lack of adequate constitutive laws, hcp sheet forming finite-element simulations have been generally performed using classical macroscopic anisotropic criteria for cubic metals. Recent advances in the formulation, numerical implementation, and validation of macroscopic plasticity models for hcp materials have allowed a better capture of specific features like the anisotropy and the tension-compression asymmetry in yielding of hcp metals.

A more relevant approach is the physically-based one, which requires a good understanding of the deformation mechanisms at the individual grain-scale in the polycrystalline sample. Moreover, depending on its orientation, the grain response involves different slip systems activity rates. Indeed, an accurate determination of slip resistance and its evolution, that is hardening, is of prime importance to well predicting the macroscopic response of a polycrystalline specimen.

This work details such approach in the case of a pure polycrystalline zinc sheet. Experimental data, issued from instrumented indentation tests performed on grains of distinct crystallographic orientations is used. Combining crystal plasticity finite element method (CPFEM) with an inverse identification, we have determined the unknown

critical resolved shear stresses. We have also investigated the orientation-dependent characteristics under complex and local loading conditions such as those involved in a nanoindentation test. Indeed, the complexity of the stress state that develops underneath the indenter depends on the geometrical characteristics of the latter and the crystallographic orientations of the grains, which can give rise to different interactions between the deformation modes.

Multiphysical simulation of aluminum panels' behaviour hit by lightning strikes

Christine Espinosa [1], Florent Grotto [1], Stéphane Vilcocq [2], Frédéric Lago [2], Thomas Montel[1], Oscar Gnangnon [1]

[1] Institut Clément Ader, Université de Toulouse, ISAE-SUAPERO, IMT MINES ALBI, UTIII, INSA, CNRS, 3 Rue Caroline Aigle, F-31400 Toulouse CEDEX 04, France

[2] DGA-Techniques aéronautiques, 47, Rue Saint-Jean, 31130 Balma, France

christine.espinosa@isae-supaero.fr

One of the main safety issues facing aircrafts is the protection against lightning strikes. Metallic aircrafts are protected against current flows because of their high electrical conductivity. However, at the arc attachment location, a serious damage may happen and even it may be developed into a perforation. Such perforation in the fuel tanks or close to the energetic materials may jeopardize the safety of the aircraft and the holding of the carriers. Laboratory tests simulating lightning strikes follow standard regulations requirements that prescribe the current waveforms the structure must resist depending on the zone of the airplane. D+B+C* current waveforms are under concern here and are reproduced in by specific current delivery devices at DGA-Ta lightning lab. Sensibility analysis done after experimental variability campaigns on aluminum panels allowed us introducing a Damage Severity Index as a quantitative representation of the severity level of the local damage [1]. Typical local damage are a dome on front face, a double dome on front and rear face, a sharp crater on front and rear face, and a hole, of typical diameters of about 10mm. The DSI showed as expected the major effect of the delivered electrical charge (in Coulombs). The second most active parameter was the position of the hit. In contrary to composite panels [2], it is surprising for metallic plate damage.

It is then of particular importance to understand the contribution of each component of the load on the global behavior of the panel during the lightning in order to understand why local damage is affected.

This talk will present the fully LS-DYNA® electromagnetic-thermal-transient mechanical coupled numerical model that has been developed to represent the D-B-C* loading. Results of numerical simulations are presented for different sets of loadings.

The contribution of each component of the load on the macroscopic panel behavior and maximum local temperature is investigated.

[1] C. Espinosa, I. Alhossen, A. Hor, E. Pierré, S. Vilcocq, R. Chieragatti, T. Montel, O. Gnangnon (2018). Experimental investigation of the repeatability of direct damage induced by lightning strikes on metallic panels. 15th High-Technology Plasma Processes (HTPP15), Toulouse, France.

[2] Y. Duval, A. Bigand (2017). Effect of boundary conditions on damage resulting from a D-waveform on a composite plate. International Conference on Lightning and Static Electrocity (ICOLSE), Nagoya, Japan.

The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics

Irina Tezaur [1,*], Alejandro Mota[1], Coleman Alleman[1], Greg Phlipot[2]

[1]Sandia National Laboratories, [2]California Institute of Technology

*ikalash@sandia.gov

Concurrent multiscale methods are essential for the understanding and prediction of behavior of engineering systems when a small-scale event will eventually determine the performance of the entire system. Here, we describe the recently-proposed [1] domain-decomposition-based Schwarz alternating method as a means for concurrent multiscale coupling in finite deformation quasistatic and dynamic solid mechanics. The approach is based on the simple idea that if the solution to a partial differential equation is known in two or more regularly shaped domains comprising a more complex domain, these local solutions can be used to iteratively build a solution for the more complex domain. The proposed approach has a number of advantages over competing multiscale coupling methods, most notably its concurrent nature, its ability to couple non-conformal meshes with different element topologies (Figure 1), and its non-intrusive implementation into existing codes.

In this talk, we will first overview our original formulation of the Schwarz alternating method for multiscale coupling in the context of quasistatic solid mechanics problems [1]. We will discuss the method's proven convergence properties, and demonstrate its accuracy, convergence and scalability of the proposed Schwarz variants on several quasistatic solid mechanics examples simulated using the Albany/LCM code.

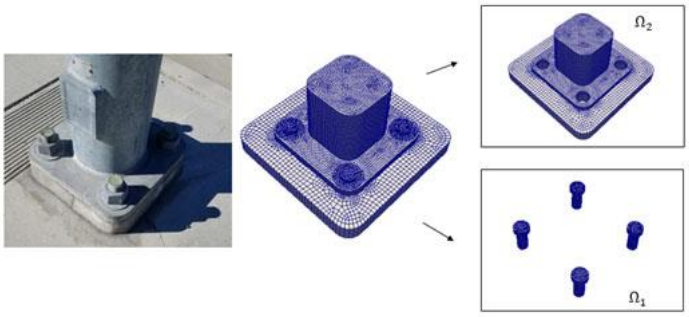


Figure 1: Schwarz Domain Decomposition for Production-Like Bolted-Joint Geometry

The bulk of the talk will present some recent extensions of the Schwarz alternating formulation to *dynamic* solid mechanics problems [2]. Our dynamic Schwarz formulation is *not* based on a space-time discretization like

other dynamic Schwarz-like methods; instead, it uses a governing time-stepping algorithm that controls time-integrators within each subdomain. As a result, the method is straight-forward to implement into existing codes (e.g, Albany/LCM), and allows the analyst to use different time-integrators with different time steps within each domain. We demonstrate on several test cases (including bolted-joint problems of interest to production; e.g. Figure 1) that coupling using the proposed method introduces no dynamic artifacts that are pervasive in other coupling methods (e.g., spurious wave reflections near domain boundaries), regardless of whether the coupling is done with different mesh resolutions, different element types like hexahedral or tetrahedral elements, or even different time integration schemes, like implicit and explicit. Furthermore, on dynamic problems where energy is conserved, we show that the method is able to preserve the property of energy conservation.

REFERENCES

[1] A. Mota, I. Tezaur, C. Alleman. "The alternating Schwarz method for concurrent multiscale coupling", *Comput. Meth. Appl. Mech. Engng.* 319 (2017) 19-51.

[2] A. Mota, I. Tezaur**,** G. Phlipot. "The Schwarz alternating method for dynamic solid mechanics", in preparation for submission to *Comput. Meth. Appl. Mech. Engng.*

Modelling of honeycomb composite sandwich panel with flax fiber skin

Matteo Riganti[1,2],Frèdèric Lachaud[1],Christine Espinosa[1], Mathieu Boutin[1]

[1] *Institut Clément Ader (ICA), Université de Toulouse, ISAE-SUPAERO, INSA, IMT MINES ALBI, UTIII, CNRS, 3 Rue Caroline Aigle, 31400 Toulouse, France*

[2] *POLITECNICO DI MILANO, Piazza Leonardo da Vinci, 32, 20133 Milano, Italia*

frederic.lachaud@isae-supaero.fr

riganti.matteo@outlook.it

A study over a flax fiber sandwich and a honeycomb/E-glass fiber sandwich (standard aeronautic sandwich cabin panel) is conducted in order to trace and compare their response behavior, under static and dynamic loads (impact). Firstly, skin and core are taken into consideration separately. For the skin, realized by fabric plies, a damage model [4] developed in precedent study [2] is applied. For Nomex® honeycomb, experimental tests are realized (fig.1) to understand overall behavior [1,3], and after the influence of geometrical local imperfections due to manufacture process, and of uncertainties in mechanical properties, is taken into account. Different FEM models (fig.2) are realized and set in order to fit experimental curves (fig.3). Through a variability analysis, mesh influence is investigate randomly displacing nodes and its consequence over instability phenomena will be evaluated, while the effect of mechanical property uncertainties is investigated using a parametrical approach.

Figure 1: Experimental crushing of Nomex® honeycomb

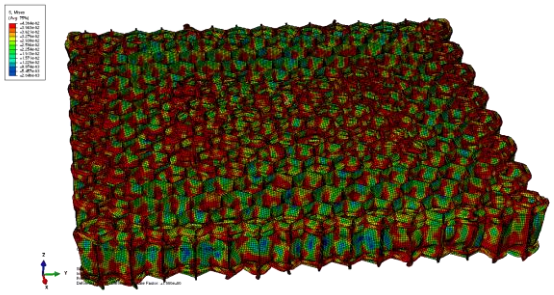


Figure 2: FEM simulation of honeycomb compression

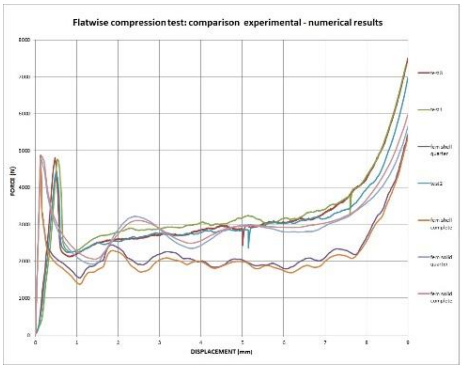


Figure 3:Experimental curve flatwise compression test

Acknowledgement: thanks to VESO-CONCEPT for materials supply.

References:

[1] M. Giglio, A. Manez, A. Giglioli, *Investigations on sandwich core properties through an experimental–numerical approach*, Politecnico di Milano, Composites: Part B 43 (2012) 361–374

[2] F. Lachaud, C. Espinosa , L. Michel ,P. Rhame, R. Piquet, *Modelling Strategies for Simulating Delamination and Matrix Cracking in Composite Laminates.* Applied Composites Materials. DOI 10.1007/s10443-014-9413-4, August 2014

[3] D. Mohr, M. Doyoyo, *Deformation-induced folding systems in thin-walled monolithic hexagonal metallic honeycomb*, MIT, U.S.A., International Journal of Solids and Structures 41 (2004) 3353–3377

[4] C.G. Skamniotis, M. Elliott, M.N. Charalambides, *On modelling the constitutive and damage behaviour of highly non-linear bio-composites – Mesh sensitivity of the viscoplastic-damage law computations*, Imperial College London, International Journal of Plasticity 114 (2019) 40–62

Probablistic approach of a dynamic analysis of wind turbine on flexible foundation

Abderraouf Kamel[1,2] . Abdelkhalak El Hami[1] . Mounir Ben Jdidia[2] . Lotfi Hammami[2] . Majdi Yangui[2]. Mohamed Haddar[2] .

[1]Laboratory of Mechanics of Normandy (LMN), National Institute of Applied Sciences of Rouen, Rouen, France.

[2]Laboratory of Mechanics, Modeling and Manufacturing (LA2MP), Mechanical Engineering Department, National School of Engineers of Sfax, Sfax, Tunisia

abderraouf.kamel @insa-rouen.fr

In this paper, a dynamic analysis of a wind turbine in flexible base is carried out and combined with a stochastic analysis to investigate the robustness of the system. Climatic properties and geotechnical properties are chosen as random variable.in fact,for this analysis, a finite element model with Matlab software of horizontal axis wind turbine rated at 500 kW is elaborated. Fig1

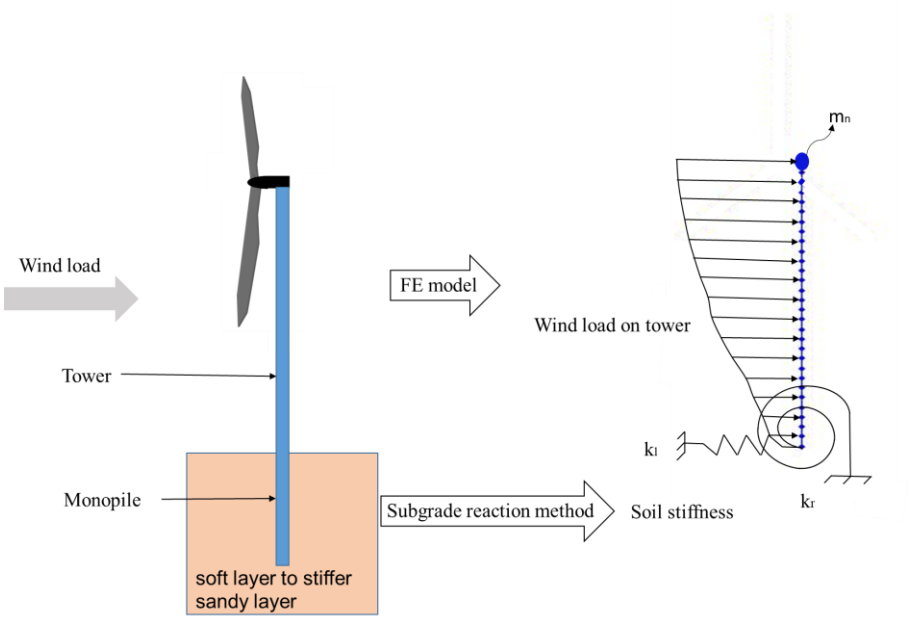


Figure 1 A the FE model of a wind turbine with monopole foundation

In this work, the tower was considered as regular column with a top mass. The properties of the turbine tower are summarized in Table 1.

Table 1 design parameters of the turbine tower

Parameters	Description	Values
D_T	tower diameter	2.5 m
e_T	tower thickness	0.012 m
E_T	Young's modulus	$2.1\ 10^{11}$ Pa
ρ_T	Mass density	7800 kg/m^3
V_{10}	the wind speed at the height 10 m	10 m/s
m_n	Mass of the nacelle	32 000 Kg
	Rated power	500 KW

Monopile is used to support this slender structure. The subgrade reaction method is used to model the soil-structure-interaction (SSI) [1].in this method, pile-soil is substituted by a lateral spring and another rotation. Wind action is then applied to the wind turbine.

Wind velocity v_{10}, lateral stiffness k_l and rotational stiffness k_θ of the foundation are chosen as random variables that will be used in the stochastic study of the system.

In this study, the results of MC simulation [2], which will be considered as a reference, are compared with that of gPC simulation [3]. It has been found that gPC simulation almost reproduces the results of MC simulations for a small standard deviation ($\sigma_{v10}= \sigma_{kl} =\sigma k_\theta =5\%$) with a second-order polynomial. For a higher standard deviation ($\sigma_{v10}= \sigma_{kl} =\sigma k_\theta =10\%$) a, six-degree polynomial is sufficient to produce accurate results.

Knowing that the gPC simulations are accompanied by a phenomenal reduction in computing time compared with MC simulations, this technique then presents an effective and powerful tool for studying the robustness of the structure for this type of problems.

References

[1] S. Adhikari et S. Bhattacharya, «Dynamic analysis of wind turbine towers on flexible foundations,» *Shock and Vibration*, vol. 19, pp. 37-56, 2012.

[2] Y. A. ,. e. Shreider, The Monte Carlo method: the method of statistical trials, vol. 87, Elsevier, 2014.

[3] D. Xiu et G. E. Karniadakis, «Modeling uncertainty in flow simulations via generalized polynomial chaos,» *Journal of computational physics*, vol. 187, n° %11, pp. 137-167, 2003.

Multi-scale Reliability Based Design Optimisation for Unidirectional FRP Composite Laminates

Sadik Omairey[1], Peter D. Dunning[1], Srinivas Sriramula[1a]

[1]School of Engineering, University of Aberdeen, AB24 3UE
[a]Lloyd's Register Foundation (LRF) Centre for Safety and Reliability Engineering, University of Aberdeen, AB24 3UE
s.omairey@abdn.ac.uk

The full benefits of FRP are often not realised in practice due to conservative safety factors arising from a lack of understanding of how uncertainties affect performance. Therefore, in this study a multi-scale reliability-based design optimisation (RBDO) framework is developed for a unidirectional fibre reinforced polymer (FRP) composite laminate. In terms of reliability, a probabilistic framework, developed by the authors (Omairey et al, 2019, Omairey et al, 2018), that employs a FEA-based surrogate model is used to estimate stiffness properties, while accounting for geometric and material property uncertainties at micro, and meso scales. Using the developed framework, lamina thickness and orientations are optimised to minimise mass, subject to reliability constraints on several stiffness criteria at the laminate scale.

Many of the uncertainties occur due to the multi-scale build-up nature of composites, mainly in material properties and geometric characteristics. These uncertainties present a challenge in estimating composite material properties and conducting reliability-based optimisation. The currently available property estimation/homogenisation tools that are used to carry out reliability analysis and optimisation are mainly divided into two categories: analytical approaches, based on an assumed model configuration, and finite element homogenisation methods that are more flexible and accurate, but computationally expensive. Hence, this study uses a surrogate model based framework utilising numerically homogenised FEA data, which is capable of representing various multi-scale uncertainties. Employing this framework significantly decreases the analysis duration compared with FEA; therefore, it is feasible to conduct multi-scale reliability analysis and reliability-based optimisation of unidirectional FRP composite laminates.

Keywords: Composites; Uncertainty; Homogenisation; Surrogates; Reliability; Optimization.

References

Omairey, S., Dunning, P. and Sriramula, S. (2019). Multiscale Surrogate-based Framework for Reliability Analysis of Unidirectional FRP Composites. Composites Part B: Engineering, [under review].

Omairey, S., Dunning, P. and Sriramula, S. (2018). Influence of micro-scale uncertainties on the reliability of fibre-matrix composites. Composite Structures, 203, pp.204-216.

Efficient structural reliability analysis based on polynomial chaos expansion and maximum entropy method

Jinsheng Wang [1] ; Muhannad Aldosary[2]; Chenfeng Li[1]

[1] Zienkiewicz Centre for Computational Engineering, Swansea University, Swansea, SA1 8EN
[2] Dams and Water Resources Engineering, University of Anbar, Iraq
844051@swansea.ac.uk

Abstract: In the presence of uncertainties, the proper assessment of the failure probability of a structural system is an important component in the modern reliability-based engineering framework. However, the estimation of failure probability of a structural system can generally be computationally demanding, especially for rare failure events where complex finite element models are involved for response evaluation. Therefore, alternative approaches for efficient computation of structural failure probability while retaining high accuracy is of paramount importance to the structural engineering community. Thus, herein this work an efficient hybrid approach is proposed that combines an efficient surrogate model technique with the maximum entropy method (MEM) for accurate failure probability evaluation of a structural system. In the proposed method, the statistical moments of the performance are furnished by the surrogate model, whereas the probability density function (PDF) is constructed using MEM under moment constraints. With the availability of the analytical expression of PDF, the failure probability of the structural system is directly obtained by numerically integrating the PDF over the failure domain. The applicability of the proposed approach is investigated using numerical examples and its performance is compared with Monte Carlo simulation (MCS) and conventional reliability analysis methods, namely first-order reliability method (FORM), importance sampling method (IS) and subset simulation (SS), whenever possible. It is observed that: the proposed method has the capability to fully and accurately capture the uncertainty inherent in the model response with a relatively small number of functional calls, which is more efficient compared with simulation approaches; the proposed method can readily provide failure probability estimation once the PDF is constructed, which is especially attractive when different thresholds are of concern; other efficient surrogate model methods, such as support vector machine, artificial neural network and Kriging, can easily be incorporated into the presented framework for structural reliability analysis, which is the scope of the future research.

Key Words: Structural reliability analysis; Surrogate model; Maximum entropy method; Statistical moments; Probability density function

Performance of drag models in CFD-DEM

Sizeng You [1], Ashutosh Bhokare[1], *Chenfeng Li[1]

[1]College of Engineering, Swansea University, UK

* Corresponding author: c.f.li@swansea.ac.uk

Flows witnessed in nature and the industry rarely involve a single phase. A thorough understanding of multiphase flows is critical to the design, up-scaling, optimisation, and correction of industrial processes. Multiphase flows in which one phase is a fluid and the other is solid-particulate finds applications in fluidised beds, cyclone separators, pneumatic conveyors and other industrial processes. This class of multiphase flows can be modelled using the Eulerian-Eulerian approach in which both the fluid and particulate phases are treated as inter-penetrating continua. Although this approach is able to model macroscopic phenomena it does not capture the local behaviour of particles. In order to accurately model particle motion an alternative Eulerian-Lagrangian approach can be used in which the fluid is treated as a continuum and the solid-particulate as discrete Lagrangian particles interacting with the continuum phase. The discrete element method (DEM) is a numerical technique which describes the motion of discrete particles by solving Newton's second law of motion. The coupling strategy of modelling fluid flow using computational fluid dynamics (CFD), particulate motion using DEM and the interaction between them is referred to as CFD-DEM.

CFD-DEM is considered to be a meso-micro approach in which the fluid phase is modelled at the mesoscopic level and the solid-particulate phase at the microscopic level. The Navier-Stokes equations are used as the governing equations for the fluid phase and can be solved using the finite volume method (FVM). Newton's second law of motion is used as the governing equation for the particles and solved using numerical techniques under DEM. In a complete two-way coupled CFD-DEM scheme the presence of solid phase is considered as a volume fraction field and the Navier-Stokes equations are modified likewise. Newton's third law of motion is obeyed by considering exchange of momentum between the phases. The drag and pressure gradient force are found to be the dominant forces. Thus, an accurate drag model is critical to the accuracy of a CFD-DEM scheme.

This talk introduces the CFD-DEM scheme and all the numerical ingredients needed to successfully implement it. It then introduces the various drag models available in literature and popularly used in CFD-DEM. To compare the performance of the drag models a problem statement is defined in which fluid is forced to flow through a region of stationary particles and the drag on the particles is computed. The results of a purely CFD simulation in which the particles are fully resolved by the FVM mesh is used as the basis of the comparison. CFD-DEM simulations are run using the drag models in the same setup and an attempt to compare their performance at various inlet velocities is made. It is found that at low Reynolds number flows, the drag models contain a constant predictable error while at higher Reynolds number flows the error builds up with the flow rate and is highly unpredictable. Although the error in drag is slightly sensitive to the volume fraction, it does not seem to affect the accuracy by a huge margin for most drag models.

PyEFEM: Massively parallel python based FEM framework for flow problems

Liang Yang [1,2]
[1]School of Water, Energy and Enviroment (SWEE), Cranfield University, Bedford, UK
[2] Department of Earth Science and Engineering, Imperial College London, South Kensington, UK
liang.yang@cranfield.ac.uk

Numerical simulations of complex multiphysics multiscale problems, such as fluid-structure interaction, turbulent flows, which demand fine spatial and temporal resolutions, require often impractical (or unavailable) computing resources. The performance in supercomputing on modern computer architectures is typically restricted by the cost of memory per core. Loading the memory is slower than the performing the arithmetic operations. The matrix-free methods, where matrix-vector product is formed on-the-fly becomes popular, including on GPUs. The Cartesian data structure is much faster than unstructured, as the structured meshes can be easily accessed by the index. Unstructured solver involves an additional cost arising from indirect addressing and non-contiguous memory access.

For these reasons, the explicit stabilised finite element is designed to be a promising algorithm for solving the nearly-incompressible, turbulent flow problems, with reduced memory costs. Implementing the method, PyEFEM is a Python based framework for solving flow problems using matrix-free stabilised finite element, which exhibits excellent scalability on current supercomputing systems for large-scale unsteady flow simulations, reaching up to 10 billion unknowns on HPCs. It is designed for massively-parallel cross-platform and its applications include turbulent flow (See Fig. 1), biological flow, aeroacoustics (See Fig. 2), environmental flow (See Fig. 3), pore scale modelling (See Fig. 4), flow through porous media (See Fig.5) and haemodynamics.

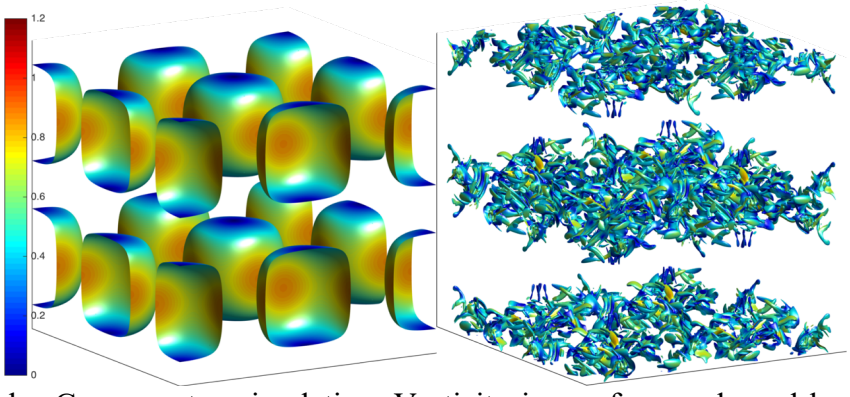


Fig. 1: Taylor-Green vortex simulation. Vorticity iso-surfaces coloured by velocity at different time instances. (left) isosurface for $|\boldsymbol{\omega}|=1$ at t=0; (right) isosurface for $|\boldsymbol{\omega}|=9$ as t=11 [1].

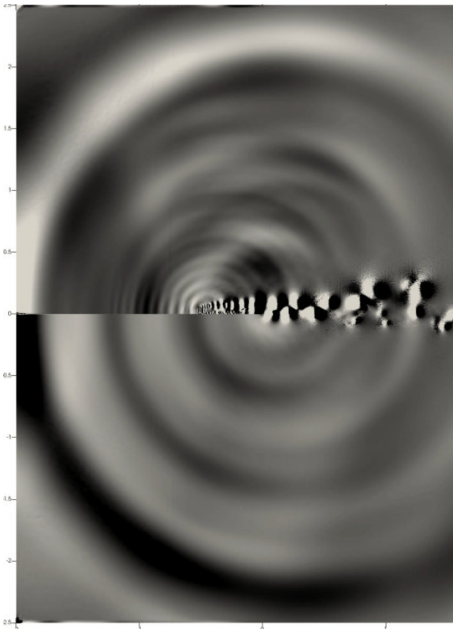


Fig. 2. Dilatation field of a flow over a trailing edge with obstacle with the non-reflecting boundary conditions (NRBCs) [2].

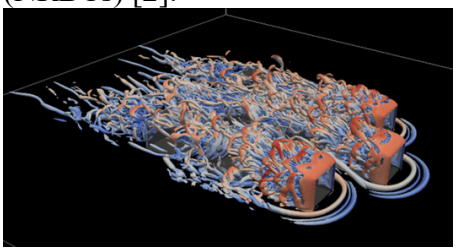


Fig. 3. Urban air flow and natural ventilation problem with PyEFEM.

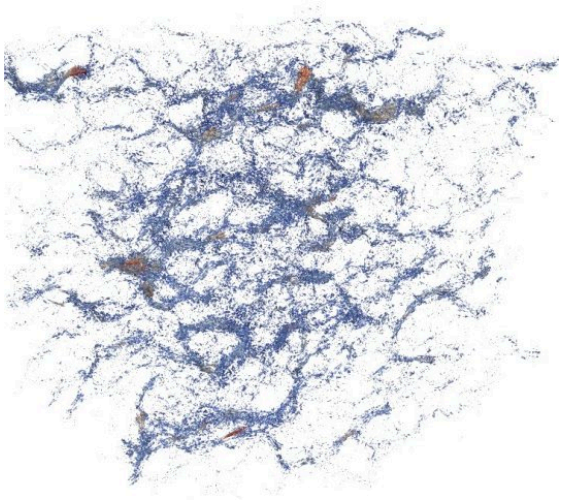


Fig. 4: Pore scale modelling, flow in Berea sandstone.

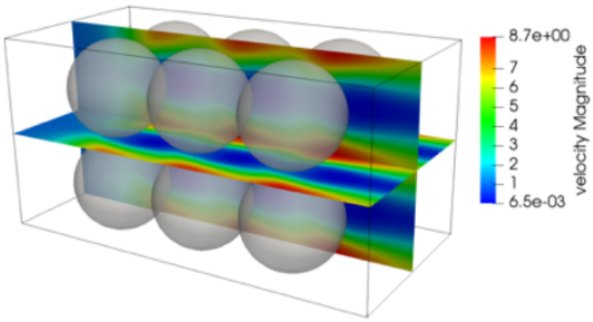


Fig. 5: Flow through a semi-infinite structured array of sphere at Re=18.

This talk will describe recent efforts at developing the matrix-free stabilised finite element models for different applications on cross-platforms. The already effective in-house research code will be taken to the next stage: a strong and versatile tool, with the application to oil & gas, nuclear thermal hydraulics, aerodynamics/noise for trains, automotive and airplanes.

References:

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

[2] Yang, L., et al. Direct numerical simulation of low Mach-number isentropic flow noise using stabilised finite element.

[3] Yang, L., Yang, J., Boek, E., Sakai, M., & Pain, C. (2019). Image-based simulations of absolute permeability with massively parallel pseudo-compressible stabilised finite element solver. Computational Geosciences, 1-13.

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
5	1.1	The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics	**Irina Tezaur** (Sandia National Laboratories)*
8	1.30	Pore Water State in Heated Concrete---Comparing a Numerical Model to NMR Measurements	**Christoph Pohl** (Bundesanstalt für Materialforschung und -prüfung)*
11	2.6	Computationally efficient homogenization for modeling of nonlinear functionally graded materials	**Witold Ogierman** (Silesian University of Technology)*
12	2.28	Multiphysics Computation in Batteries Involving Electromagnetism and Thermomechanics	**Bilen Emek Abali** (TU Berlin)*
18	1.2	On modeling interfaces in composite with multi-physic coupling	**Michele Serpilli** (Università Politecnica delle Marche
20	1.15	Sub-Modeling Approach to Investigate the Cracking Behavior of Reinforced Concrete Structures Considering Polymorphic Uncertainty	**Katharina Kremer** (Ruhr University Bochum)
25	1.7	A computational multi-physics model to predict the chemo-mechanical degradation of historical oil paintings	**Emanuela Bosco** (Eindhoven University of Technology)*
26	1.30	A coupled chemo-mechanical model for biogenic sulfide corrosion in concrete sewer pipes	**Emanuela Bosco** (Eindhoven University of Technology)*

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
27	**1.28**	Degradation of Lithium-Ion Batteries in Aerospace	**Linda J. Bolay** (German Aerospace Center)
28	**1.16**	Reduced-order Modelling Scheme for Problems with Fully Resolved Microstructures Generated by Generalized Periodic Unit Cells	**Martin Doškář** (Czech Technical University in Prague)
31	**1.13**	Fragment size characterization for granular flow in highly damaged ceramics	**Lori Graham-Brady** (Johns Hopkins University)
37	**1.5**	Development of a modified Voronoi's tesselation algorithm for the determination of the effective properties of cork-based composites	**Marco Delucia** (I2M - Institut de mécanique et d'ingénierie - Université de Bordeaux)
39	**3.13**	Data driven computational analysis of open foam materials	**Nanda Gopala Kilingar** (University of Liege)*
41	**1.4**	Simulation Model for Single unit Warpage of Shadow moire in Flip-Chip Process	**Wan-Chun Chuang** (Department of Mechanical and Electromechanical Engineering, National Sun Yat-sen University)
42	**1.19**	Efficient and accurate two-scale FE-FFT-based prediction of polycrystalline material behavior at finite strains	**Christian Gierden** (Institute of Applied Mechanics, RWTH Aachen University)
43	**1.3**	Diffusion-Kinetic Monte Carlo Methods for Neutral	**Bert Mortier** (KU Leuven)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
		Transport in Plasma Edge Simulations of Nuclear Fusion Reactors	
44	**1.6**	Development of a simple ergodic stochastic representative volume element for heterogeneous materials with random geometry of microstructure	**Dmytro Pivovarov** (Chair of Applied Mechanics, Friedrich-Alexander University Erlangen-Nürnberg)
46	**3.3**	Multi-uncertainty analysis of the indentation process of key engineering materials	**Thiago Doca** (University of Brasília)
47	**3.1**	Adjoint Based Optimisation of an Internal Cooling Channel U-Bend	**Jens-Dominik Müller** (Queen Mary, University of London)
205	**Plenary Session**	Multi-scale and Multi-physics challenges for Future Aircraft: A Hierarchical Approach	**Paul G. Tucker** (Cambridge University)
202	**2.29**	Examining the Mutation Effect of SLC26A4 STAS Domain By Observing the Communication Between Secondary Structures	**Hyun Joon Chang** (Korea University);
~~**208**~~	-	~~Probabilistic Design Optimization for CO2 Storage with Leakage Risk Control~~	~~**Ben Mansour Dia** (CPG)*~~
210	**3.11**	Development of Multiscale Multi-physics Based Modelling and Simulations with the Application to	Yizhi Shao (Brunel University)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
		Precision Machining of Aerofoil Structures	
211	3.16	An Investigation of stepwise Crack Tip Advancement	**Yanan Sun** (Swansea University)
212	3.9	Dynamic Analysis of a Multi-Contact Problem Using Simplified Models to Study of the Influence of Clearances on Contact Forces	**Victor BLANC** (French Atomic and Alternatives Energies Commission)
215	2.8	Two-scale phase field modeling of damge and fracture for disordered media	**Ye Feng** (Tongji University)
216	3.17	The Refined Algrithm of Generalized Probability Density Evolution Equation Based on Reproducing Kernel Particle Method	**Dan Wang** (Tongji University)
218	1.23	Data-Drive Approaches in Predicting Premixed Reactive Flow	**Mohsen Ayoobi** (Wayne State University)
219	2.27	Comparisons of direct numerical simulation and penalized models to compute the flow in a porous-fluid system	**Charles-Henri C.H. Bruneau** (University of Bordeaux)
220	1.20	Machine Learning-based Approach for Predicting Defects under Uncertainty in Sheet Metal Forming Processes	**Pedro Prates** (University of Coimbra)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
222	2.25	Quantified Relationship between Properties of Fresh Self-compacting Concrete and Workability Test Performance	**Sizeng You** (Swansea University)
223	1.27	Robust Flame Frequency Response Identification via a Multi-Fidelity Approach	**Shuai Guo** (Technical University Munich)
221	1.11	On the universality of the Strouhal law for High Reynolds number bluff bodies with flow control	**Avraham Seifert** (Tel Aviv University)*
224	3.6	Numerical modelling of the uncertainties in hip prosthesis material parameters	**Abdelkhalak El Hami** (INSA Rouen)
226	1.22	Multi-scale Numerical Simulation of Reinforced Concrete Framed Structure	**Xiangling Gao** (Tongji Universiry)
227	2.21	Multiscale Moddeling of Self-Affine Rough Contact	**António M Couto Carneiro** (INEGI); (Faculty of Engineering University of Porto);
228	2.24	Multi-scale adaptive unstructured mesh predictive modelling for environmental problems	**Fangxin Fang** (Imperial College London)*
229	2.17	A Global-Local Zooming Technique	**Matthias Birner** (Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
230	**1.10**	Multiscale prediction of powder properties during pressure-assisted sintering	**Szymon Nosewicz** (Institute of Fundamental Technological Research of the Polish Academy of Sciences)
231	**1.9**	Virtual material characteriazation across scales and physics: case studies	**Anna Matveeva** (Siemens Industry Software NV)
232	**2.11**	Heat transfer partitioning models for nucleate boiling	**Robin Kamenicky** (University of Strathclyde)*
233	**2.19**	A fully coupled electromagnetic-thermal-transient mechanical simulation of the load suffered by aeronautical composite panels during lightning strikes	**Christine Espinosa** (Institut Clément Ader)
234	**1.18**	Modelling of shear bands in fluid saturated poroplastic solids with embedded strong discontinuities	**Mijo Nikolic** (University of Split)
235	**1.29**	Comparison of Two New Methods for Fatigue Reliability Analysis	**Ruofan Gao** (Tongji University)
236	**2.16**	Construction of optimal basis functions in the Partition of Unity Method and their verification in complex simulations	**Denis Düsseldorf** (University Of Bonn)
238	**3.15 (presented by:**	Metamodels for RBDO of wire bonding in microsystem packages	**Abdelkhalak El HAMI** (INSA Rouen)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
	Abdelkhalak El Hami)		
241	**1.24**	New Method for Numerical Calibration of a Rotary Kiln Model - A Multiscale Approach	**Christian Jordan** (TU Wien/Institute of Chemical Engineering)
242	**1.21**	Nanoscience applied to oil and gas technologies: a multiscale computational approach	**Caetano R Miranda** (Universidade de Sao Paulo)
243	**2.18**	Designing phononic crystal with anticipated band structure through a deep learning based data-driven method	**Zhanli Liu** (Tsinghua University)
244	**2.1**	Stochastic Finite Element Analysis of U-Shaped RC Shear Wall with a Novel Random Field Modeling Strategy for Open Thin-Walled Structural Members	**De-Cheng Feng** (Southeast University)
247	**3.7**	A Turbulence Based Sensitivity Study on Drag Prediction of the NASA Common Research Model Aircraft	**Sule Ozturk** (Istanbul Technical University)
246	**1.17**	Increased Modelling Demands by Moving from Resolved to Unresolved Simulation of Heterogeneous Reactive Systems	**Bahram Haddadi Sisakht** (TU Wien))

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
250	1.8	Assessment of the Size of the Representative Volume Element of Random Heterogeneous Materials	**Pawel Holobut** (Institute of Fundamental Technological Research, Polish Academy of Sciences)
248	2.5	Approximation of frequency response functions with the multi-element generalised polynomial chaos method	**Prem Ratan Mohan Ram** (TU Braunschweig)*; Ulrich Roemer (TU Braunschweig)
251	3.19	Scaling procedure for the design of a validation experiment on an accidental gas release	**Alberto Moscatello** (Politecnico di Torino)
237	2.4	A Vibrational study of graphene sheets, carbon nanotubes, and nanocones	**Reza Ghaffari** (Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University)
252	3.10	A DFT study of single layer blue phosphorus and its implementation in a continuum model	**Farzad Shirazian** (Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University)
253	2.9	A Fully Second-Order Homogenisation Model for the Analysis of Multi-Phase Materials at Finite Strains	**Igor André Rodrigues Lopes** (Faculty of Engineering University of Porto)
254	3.14	Ductile failure analysis in metallic materials through computational homogenisation	**Rui Coelho** (Faculty of Engineering University of Porto)

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
255	**3.5**	Computational Aspects on the Constitutive Modelling of Multiphase Alloys	**Miguel V Carvalho** (Faculty of Engineering of the University of Porto)
256	**2.3**	A Finite-Strain Elasto-Viscoplastic Model for Rubber Toughened Glassy Polymers: Formulation and Validation	**Bernardo Proença Ferreira** (Faculty of Engineering University of Porto)
259	**3.8**	PGD based domain decomposition method applied to parameterized seismic models	**Prattya Datta** (BSC)
261	**2.14**	Fully coupled multi-scale finite element analysis of TRIP-assisted multi-phase alloys	**Daniel de Bortoli** (Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI)
249	**3.18**	Optimization of Control Parameters for an Electrified Vertical Take-off Landing Vehicle Using the Integral Squared Method	**Ibrahim Cicek** (Istanbul Technical University)
263	**2.23**	Multiscale stochastic simulations using a MFH model constructed from full-field SVE realizations	**Juan Manuel Calleja** (ULiege)
264	**2.2**	Simulation of adhesive squeeze flow using smoothed particle hydrodynamics	**Lorraine Aparecida Silv**a (Institut Clément Ader)
262	**2.12**	Computational methods for hybrid multiscale modelling in immunology	**Dmitry Grebennikov** (MIPT);

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
265	2.19	A Thermo-Mechanically Coupled Cutting Simulation of Ti-6Al-4V Using Advanced Meshless Methods	**Mohamadreza MA Afrasiabi** (ETH Zurich)
266	2.10	Multiphysics Simulation of Laser Metal Deposition Manufacturing Process Using a Meshless Method	**Boussad Abbès** (University of Reims Champagne-Ardenne)
267	3.4	Micromechanical Modeling and Estimation of Elastic Properties of Pure MXene (Ti3C2Tx) Films	**Shreyas Srivatsa** (AGH University of Science and Technology)
268	2.22	Computational study of deformation mechanisms in hcp metal: Application to pure zinc	**Fazilay ABBES** (University of Reims Champagne Ardenne)
269	2.7	Multiphysical simulation of aluminum panels' behaviour hit by lightning strikes	**Florent Grotto** (ICA)
270	2.13	Modelling of honeycomb composite sandwich panel with flax fiber skin	**Matteo Riganti** (ISAE-SUPAERO)
271	3.12	Presented by Abdelkhalak El HAMI: Probablistic approach of a dynamic analysis of wind turbine on flexible foundation	**Abderraouf KAMEL** (INSA Rouen)
213	1.25	A phase-field damage model with micro inertial effect for dynamic failure of quasi-brittle materials	**Lu Hai** (Tongji University);
273	2.30	Multi-scale Reliability Based Design Optimisation for	**Sadik L. Omairey** (University of Aberdeen);

PAPER ID	PRESENTATION NUMBER	PAPER TITLE	PRESENTER
		Unidirectional FRP Composite Laminates	
204	**2.15**	New Vortex Identification Methods for Tuebulence - Omega, Liutex/Rortex, Omega-Liutex	**Chaoqun Liu** (University of TexaS AT aRLINGTON)
202	**2.29**	Examining the Mutation Effect of SLC26A4 STAS Domain By Observing the Communication Between Secondary Structures	**Sungsoo Na** Korea University
277	**2.21**	277 Performance of drag models in CFD-DEM	**Ashutosh Bhokare** (Swansea University)
276	**3.2**	276 Efficient structural reliability analysis based on polynomial chaos expansion and maximum entropy method	**Jinsheng Wang** (Swansea University)
278	**2.26**	PyEFEM: Massively parallel python based FEM framework for flow problems	**LIANG YANG** (Cranfield University)
201	**1.14**	System time-variant reliability-based structural design optimization of deteriorated truss bridges	**Younes Ya Aoues** (Normandie Université, INSA Rouen Normandie, LMN)