Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems

https://cm3p.org/

—

CM3P Conference 2025 Proceedings

About

Over the past two decades, there has been a notable surge in interest surrounding the advancement of multi-physics, multi-scale and multi-uncertainty models. This surge can be attributed to the emergence of new mathematical formulations and numerical solution strategies, coupled with the escalating computational power-to-cost ratio. These factors have collectively contributed to a remarkable expansion within this dynamically evolving field.

The research landscape in this domain has focused extensively on formulating and integrating various analytical tools, such as homogenization and asymptotic analysis, alongside leveraging advanced computational methods like parallel computing, stochastic analysis, and code coupling. The application of these tools and methods spans a wide array of fields, including but not limited to metal processing, composite materials, oil and gas development, fuel cell technology, and biomedical tissue engineering. This diversification underscores the versatility and applicability of the developed models.

Significantly, these advancements have played a pivotal role in deepening our comprehension of the intricate interactions inherent in multi-physics and multi-uncertainty phenomena occurring across diverse scales in both space and time. The synergy of novel mathematical frameworks, innovative numerical approaches, and the increased efficiency of computational resources has propelled this field into a central position, fostering breakthroughs and insights across a spectrum of scientific and engineering disciplines. In the most general format, the CM3P conference targets the latest advances in the M3 fields, including the following (not exhaustive) research topics:

- Computer simulation of multi-physics processes/systems

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

- Computational homogenization and multi-scale modelling
- Stochastic modelling, probabilistic engineering, reliability and risk assessment
- Computational coupling strategies
- High-performance computing related to the M3 (multi-physics, multi-scale and multi-uncertainty) challenges
- Relevant scientific and industrial applications
- Other related topics

Chairs

Prof. Chenfeng Li FLSW
Swansea University, United Kingdom

Prof. F.M. Andrade Pires
University of Porto (FEUP), Portugal

Abstract

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

A multi-physics model for the simulation of a cold breakdown plasma and its interaction with dielectric surfaces

Andrea Villa[1,*], **Giacomo Buccella**[1], **Beatrice Crippa**[2], **Damiano Fasani**[1] [1]Ricerca sul Sistema Energetico (RSE), E-mail: andrea.villa@rse-web.it

[1]Ricerca sul Sistema Energetico (RSE), E-mail: giacomo.buccella@rse-web.it

[2]MOX, Department of Mathematics, Politecnico di Milano: beatrice.crippa@rse-web.it

[1]Ricerca sul Sistema Energetico (RSE), E-mail: damiano.fasani@rse-web.it

Abstract: In this paper, we describe an approach for the simulation of cold breakdown plasma interacting with dielectric surfaces. This model has many applications to several technological fields, such as plasma medicine [2] and surface treatments [3]. However, in this work, we mainly deal with applications to electrical engineering [10]. In fact, insulating parts of electrical components, as they age, can develop internal voids, known as treeing structures [6]. This is a very complex phenomenon where small-scale plasma discharges, also known as partial discharges [1], form inside these voids causing the propagation of the treeing. In other words, a dielectric material and the plasma void interact exchanging

mass, energy and electrical charges through an interface between the solid and the gas. Cold plasma modeling is complex in itself, as this phenomenon presents several different scales: the typical speed of electrons in these types of plasma is often 100 times greater than that of ions, and ions move much faster than neutral particles [5].

In this paper we introduce a multi-physics model to describe the interaction of a breakdown plasma with dielectric surfaces and we briefly discuss the numerical techniques that can be used to tackle it. Several physical aspects have been considered: plasma has been modelled as a reactive gas in a non-equilibrium thermodynamic state. We consider four families of species: electrons, negative ions, positive ions and neutral particles. Each family may have several species and we have included chemical models that contain, overall, more that 60 species and 600 chemical reactions [9]. Charged particles dynamics is influenced by the electric field through a drift-diffusion model. The electric field is computed with an electrostatic equation and this create a coupling between the motion of the particles and the electric field: the position of charges influences the electric field, and the electric field influences particle drift. We have also taken into account the photo-ionization: the quench of excited particles can generate photons with a sufficient energy to ionize other atoms [4]. The dynamics of neutral particles is described through Euler's equations of gasdynamics and we have also taken into account the heat diffusion. In the solid phase, we account for heat propagation and the electric field. Proper matching conditions are enforced at the interface between gas and solid domains. Another very important aspect is the modelling of the surface separating gas and solid as these two domains exchange energy, charge, and mass.

Let us introduce briefly some of the main problems that arise when discretizing the above mentioned model. The high mobility of electrons imposes a limit on the maximum time step, which is proportional to the plasma relaxation time and can be very small. Some proper implicit schemes must be adopted to achieve methods that are stable regardless the time step used [8]. Another major problem is that, where the electric field is high enough, electrons are multiplied in the plasma due to impact ionization. This is modelled by a positive reaction terms, which can cause numerical challenges by limiting both the maximum time step and mesh spacing. Some proper numerical technique have been developed, for instance, in [7] to avoid these constraints.

In this work, we employ a time-splitting method to separate the chemical model from the drift-diffusion of charged species (coupled with electrostatics) and from the dynamics of neutral particles. Our goal is todevelop a 3D simulator that reduces computational burden as much as possible while remaining stable for very large time steps. We will also discuss some test cases that have been used to validate our approach and applications to some technically relevant cases.

Keywords: Cold Plasma, Breakdown Plasma, Partial Discharges, Treeing

---

* Presenting author

References

[1] R. Bartnikas. Partial discharges. their mechanism, detection and measurement. *IEEE Transactions on Dielectrics and Electrical Insulation*, 9(5):763–808, October 2002.

[2] Gregory Fridman, Gary Friedman, Alexander Gutsol, Anatoly B. Shekhter, Victor N. Vasilets, and Alexander Fridman. Applied plasma medicine. *Plasma Processes and Polymers*, 5(6):503–533, August 2008.

[3] S.L. Kaplan and P.W. Rose. Plasma surface treatment of plastics to enhance adhesion. *International Journal of Adhesion and Adhesives*, 11(2):109–113, April 1991.

[4] Ningyu Liu, S´ebastien C´elestin, Anne Bourdon, Victor P. Pasko, Pierre S´egur, and Emmanuel Marode. Application of photoionization models based on radiative transfer and the helmholtz equations to studies of streamers in weak electric fields. *Applied Physics Letters*, 91(21), November 2007.

[5] R Morrow and J J Lowke. Streamer propagation in air. *Journal of Physics D: Applied Physics*, 30(4):614–627, February 1997.

[6] A. Villa, G. Buccella, L. Barbieri, D. Palladini, G. D'Avanzo, and R. Schurch. About plasma-polymer interaction and treeing progression. In *2024 IEEE 5th International Con- ference on Dielectrics (ICD)*, pages 1–4. IEEE, June 2024.

[7] Andrea Villa, Luca Barbieri, Marco Gondola, Andres R. Leon-Garzon, and Roberto Malgesini. Stability of the discretization of the electron avalanche phenomenon. *Journal of Computational Physics*, 296:369–381, September 2015.

[8] Andrea Villa, Luca Barbieri, Marco Gondola, and Roberto Malgesini. An asymptotic preserving scheme for the streamer simulation. *Journal of Computational Physics*, 242:86– 102, June 2013.

[9] Andrea Villa, Luca Barbieri, Gondola Marco, Roberto Malgesini, and Andres R Leon-Garzon. Simulation of the ac corona phenomenon with experimental validation. *Journal of Physics D: Applied Physics*, 50(43):435201, September 2017.

[10]

Andrea Villa, Giacomo Buccella, Luca Barbieri, Daniele Palladini, and Giovanni D'Avanzo. A multi-resolution method for internal partial discharge simulation. *Journal of Computational Physics*, 491:112362, October 2023.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

An *In Vivo* Image-Based Multiscale Framework for Mechanical Characterization of Bone Tissue

Yunhua Luo [1,2,a]

[1] Department of Mechanical Engineering, University of Manitoba, Winnipeg, Canada.

[2] Deaprtemnt of Biomedical Engineering, University of Manitoba, Winnipeg, Canada.

E-mail: Yunhua.Luo@umanitoba.ca

Hip fracture caused by falls is a common health problem among the elderly worldwide due to the prevalence of osteoporosis. Clinicians often use bone mineral density (BMD) as a surrogate for bone strength to assess hip fracture risk, but this approach has been shown to be unreliable and inaccurate. From a material mechanics perspective, hip fracture risk is determined by both the strength of the affected bone and the impact force induced by the fall, both of which are subject-specific. Therefore, accurately characterizing individual bone strength is crucial for hip fracture assessment, as it is influenced by factors such as age, gender, and overall bone health. Bone strength is determined by its chemical composition and microstructure, both of which must be accurately characterized to evaluate bone strength effectively. Advanced medical imaging techniques, such as quantitative computed tomography (CT) and dual-energy computed tomography (DECT), offer non-invasive methods for acquiring detailed information about bone chemical composition and microstructure. However, despite extensive research in image-based mechanical characterization of bone tissue, the relationship between bone mechanical properties and imaging data is often oversimplified. This paper presents a multiscale

framework utilizing DECT-acquired information for the mechanical characterization of bone tissue.

Bone has a complex chemical composition, but from a composite material perspective, it can be classified into three primary components: inorganic minerals (mainly hydroxyapatite), organic proteins (mainly type I collagen), and water. Since water exists in both free and bound forms, which are difficult to distinguish using medical imaging, a more practical classification of bone composition is into inorganic and organic components [1].

The bone material information captured in CT images reflects multiscale heterogeneity. At the sub-voxel scale, each voxel contains varying fractions of organic and inorganic content, resulting in differences in grayscale intensity between voxels. At the voxel scale, a constant intensity is assigned to each voxel during CT scanning, necessitating homogenization techniques to determine the effective material properties for a group of voxels. At the bone level, when voxel-based finite element analysis (FEA) becomes computationally prohibitive, a coarser finite element mesh is used, requiring accurate determination of material properties at the element level. These multiscale characteristics must be carefully considered to capture the true mechanical behavior of bone and ensure reliable predictions of its strength and fracture risk.

While single-energy CT can capture bone microstructure, it cannot provide information about bone composition. Dual-energy computed tomography (DECT), however, enables the characterization of inorganic and organic content in bone by exploiting the differences in their

[a] Presenting Author

linear attenuation coefficients. Figure 1 illustrates the framework for the mechanical characterization of bone tissue based on DECT.

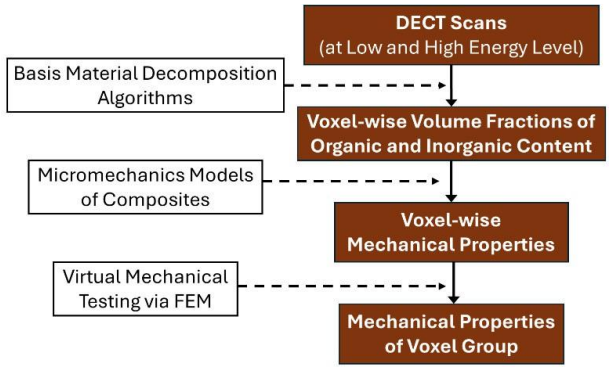
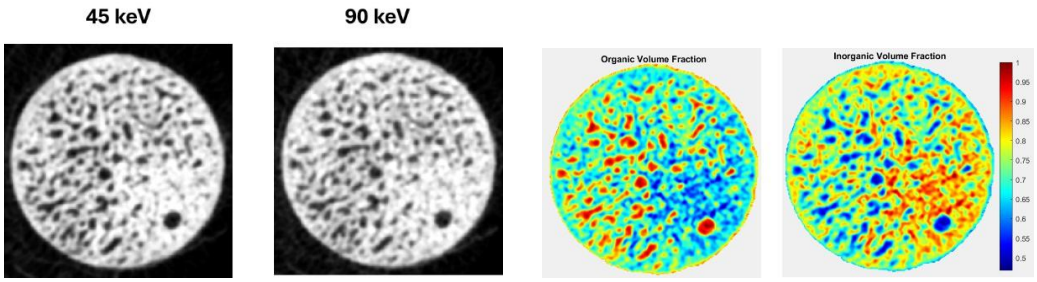


Figure 1 Multiscale framework for mechanical characterization of bone tissue

Bone CT scans are acquired at low and high energy levels (Figure 2(a)). Basis material decomposition algorithms are then applied to determine the volume fractions of organic and inorganic content (Figure 2(b)). Micromechanical models for composite materials, such as the Generalized Self-Consistent Scheme or the Mori-Tanaka method, are used to determine the bone properties for each voxel. To obtain the mechanical properties of a group of voxels, virtual mechanical testing based on finite element modeling (FEM) with appropriate boundary conditions can be employed [2]. This group of voxels can represent either a voxel-based finite element model of the entire bone or a subdomain around a Gaussian integration point within an element when a coarser finite element mesh is used to simulate the bone.



(a) (b)

Figure 2 Characterization of bone organic and inorganic content using DECT images. (a) CT scans at low and high energy level. (b) Characterized volume fractions of organic and inorganic components.

Keywords: Multiscale mechanical characterization; Dual-energy computed tomography (DECT); Bone strength; Finite element modeling; Basis material decomposition.

Reference

[1] Y. Luo and X. Wu, "Bone quality is dependent on the quantity and quality of organic- inorganic phases," *Journal of Medical and Biological Engineering*, vol. 40, pp. 273–281, 2020.

[2] Y. Luo, "Microstructure-free finite element modeling for elasticity characterization and design of fine-particulate composites," *Journal of Composites Science*, vol. 6, p. 35, 2022.

Sequential and Iterative Method for Flux-linked Scalar Transport Equations in Multi-Physics Multi-Region Problems

Raviteja Yakkala [1,a], Sreenivas Jayanti [1]

[1] Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India, 600036. E-mail: ch22d406@smail.iitm.ac.in, sjayanti@iitm.ac.in

Accurate modeling of multi-physics problems in systems poses significant computational challenges, especially when one has to deal with coupled transport phenomena across interfaces of multi-domain system featuring significant differences in geometric complexity and flow physics. Many of the electrochemical units underpinning the present trend towards harnessing renewable energy, such as fuel cells that produce electricity using hydrogen, electrolyzers that produce hydrogen using electricity and flow batteries that store electrical energy, fall in this category of engineering systems. Building a robust simulation platform that accounts for all geometrical physic-chemical aspects of these devices is a daunting task. It is necessary to take account of, and optimize, flow, thermal and electrochemical phenomena occurring in different scales, different regions and subject to different laws and constraints of physics. Against this background, we propose a sequential and iterative method for flux-lined scalar transport equations (SIMFLiSTE) for solving such complex multi-physics problems encountered in electrochemical engineering applications. In this approach, the computational domain is divided into sub-regions (which may in some cases overlap) with some shared boundaries. The flow physics of each region is governed by its own set of scalar transport equations: the transport coefficients, source terms and/or some boundary conditions applicable in each region may be governed by what happens in other regions, thereby necessitating flux transport between

regions. The governing equations of the entire system spanning across multiple regions are therefore solved independently, sequentially and iteratively until convergence.

In the present work, we illustrate the application of SIMFLiSTE approach to the improved design of inlet and outlet headers of a high temperature polymer electrolyte (PEM) fuel cell for optimal electrochemical performance of cell. Typical PEM fuel cell simulation requires computing fluid flow of the reactant and the product species in the flow channels and gas diffusion layers (GDL), transport of electronic and ionic species in the membrane-electrode-assembly (MEA) region and beyond, as appropriate, and heat transport over the entire domain by conduction and convection. The local current distribution, which is of ultimate interest, is dependent on all these phenomena. Using the SIMFLiSTE approach, we capture, through a coupled simulation of the anode side, the cathode side flow fields and the MEA, how the inlet/outlet header design influences the electrochemical performance the cell. The proposed methodology thus enables scalable and efficient simulation of this multi-physics, multi-domain system so that optimal designs can be explored.

Keywords: Computational fluid dynamics, multi-physics problems, electrochemical application, boundary flux-linked domains, coupling algorithm, PEM fuel cell

VEPD Model in Meso-Scale Approach

Gianluca Mazzucco1,*, Beatrice Pomaro1, Jiangkun Zhang1, Valentina Salomoni1

[1]Department of Civil, Environmental and Architectural Engineering (DICEA)

University of Padova (UNIPD) Via F. Marzolo 9, 35131 Padova, Italy. e-mail: gianluca.mazzucco@unipd.it.

Abstract: Building materials like cement concrete or asphalt concrete are highly heterogeneous composites. However, they are often treated as homogeneous media when a sufficiently large Representative Elementary Volume (REV) is defined. While this homogenized approach simplifies modeling, it fails to capture the interactions between different material phases. To address this limitation, a meso-scale approach has recently gained attraction. This method allows for the explicit representation of the principal material components within the REV, enabling a more detailed study of composite or conglomerate materials. At the meso-scale, local interactions between inclusions and the matrix can be analysed, revealing complex triaxial stress states under loading [1]. Concrete materials, at the meso-scale, can be modelled as three-phase heterogeneous media, consisting of coarse aggregates, a matrix, and the Interfacial Transition Zone (ITZ) between the matrix and the inclusions [2]. Meso-scale modeling requires accurate reconstruction of the material geometry and sophisticated material descriptions. Geometry can typically be obtained through industrial tomography or by using random distribution algorithms designed to replicate the correct grading curve. In this study, we propose a Visco-Elasto-

Plasto-Damage (VEPD) model to evaluate the behaviour of concrete materials under various loading conditions. Different approaches to geometry reconstruction are also explored to assess their impact on the results.

Keywords: creep, plasticity, damage, meso-scale, concrete

---

* Presenting author

References

[1] G. Mazzucco, B. Pomaro, V. A. Salomoni, C. E. Majorana 2024. Three-dimensional meso-scale modeling of asphalt concrete. Comput. Struct., 305, 107535.

[2] G. Mazzucco, V.A. Salomoni, C. Majorana 2021 A cohesive contact algorithm to evaluate the mechanical behaviour of concrete ITZ at different roughness conditions. Con- struction and Building Materials, 294, 123479.

Computational methods in nondestructive evaluation at concrete floors in multisite facilities.

Mateusz Moj [1*] , Sławomir Czarnecki [1,a] Łukasz Sadowski [1,b]

[1] Department of Materials Engineering and Construction Processes, Wroclaw University of Science and Technology, Poland, E-mail[*]: mateusz.moj@pwr.edu.pl

The costs associated with concrete flooring for large-scale industrial and warehouse facilities can comprise as much as one-fifth of the total costs associated with the project. Due to the high costliness of the stage, the requirements for the proper execution of the concrete element most exposed to a variety of functional loads are also very high. To make sure that the functional parameters meet these requirements, a wide range of tests should be used to evaluate the element - mainly based on destructive methods.

Due to the dynamic development of machine learning techniques, their ways of application are also multiplying in the surface evaluation of concrete elements [1]. The undoubted advantage of their use in the construction industry is the possibility of increasing the accuracy of non-destructive methods that allow non-invasive analysis of the parameters responsible for the comfortable and safe use of industrial floor. Researchers recommend, especially in complex matters, a combined approach to increase the performance indicators of predictive models [2].

The use of ML model-assisted NDT methods brings many advantages over traditional destructive methods [3]. An example of this comparison is the pull-off method, in which it is necessary to take at least 1 measurement per 3 m^2 of floor, which for a 25 x 120 m hall results in 1000 measurements. The time frame for such

an undertaking can require up to two months of implementation and the activities themselves cause local damage requiring repair. Abrasion

---

[a] Presenting Author

References:

[1] W. Ye, H. Huang, B. Zhang, Y. Liu, Z. Lin. 2024. Lightweight concrete crack detection based on spiking neural networks. *Engineering Computations*, *41*(10), pp. 2534-2548.

[2] S. K. Dwivedi, M. Vishwakarma, A. Soni. 2018. Advances and researches on non destructive testing: A review. Materials Today: Proceedings, 5(2), pp. 3690-3698.

[3] M. Moj, S. Czarnecki, Ł. Sadowski. 2024 Recent Trends in Using Artificial Intelligence in Evaluating Functional Properties of Industrial Concrete Floors, Proceedings of the 15th International Conference on Computational Structures Technology, Online vol.: CCC 9, p.14.2. [b] Presenting Author

References:

[1] W. Ye, H. Huang, B. Zhang, Y. Liu, Z. Lin. 2024. Lightweight concrete crack detection based on spiking neural networks. *Engineering Computations*, *41*(10), pp. 2534-2548.

[2] S. K. Dwivedi, M. Vishwakarma, A. Soni. 2018. Advances and researches on non destructive testing: A review. Materials Today: Proceedings, 5(2), pp. 3690-3698.

[3] M. Moj, S. Czarnecki, Ł. Sadowski. 2024 Recent Trends in Using Artificial Intelligence in Evaluating Functional Properties of Industrial Concrete Floors,

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Proceedings of the 15th International Conference on Computational Structures Technology, Online vol.: CCC 9, p.14.2.

resistance test methods similarly require interference with the test item. Suggestions to replace destructive methods with a hybrid combination of NDT and AI-based computational methods will allow: multiple measurements, no need for intake repairs, reduced evaluation time, and high predictive accuracy.

Funding information

Authors received funding from the National Science Centre, Poland under project PRELUDIUM 23 number 2024/53/N/ST8/00451.

Keywords:

Concrete floors, Nondestructive methods, Machine learning, Multiscale evaluation.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Effect of Correlation and Nonlinearity on Uncertainty in the Response from Computational Simulation Models

TERJE HAUKAAS[1]

[1] The University of British Columbia, Vancovuer, Canada, E-mail: terje@civil.ubc.ca

This paper has three objectives. The first is to expose the effect of correlation, in the context of nonlinearities that exist in computational simulation models. In this regard, it is nonlinearity in the parameter-response relationships that matters, not nonlinearity in the load- response relationship. In other words, the presented developments are valid for both linear and nonlinear structural analysis. The second objective is to uncover and explain what makes different models equivalent, in the context of uncertainty quantification. Specifically, models for nonlinear material behavior are compared. While the considered models are equivalent from a deterministic perspective, stringent requirements are spelled out in order for the models to be equivalent in terms of the modeling of uncertainty. A byproduct of this work is revealing how the response uncertainty vary with model granularity. The third objective is to put forward new response sensitivity vectors to rank the relative influence of the coefficient of variation of the input variables on the mean and coefficient of variation of the response.

The presented work builds upon several premises. First, repeated sampling is avoided in favor of learning as much as possible from each individual run of the computational simulation model. Second, exact response sensitivities are calculated in an efficient manner using the direct differentiation method. The author's previous work, including studies at UC Berkeley and the present professorship in Canada, includes new developments for that method. Both first-

and second-order derivatives are explored in this paper. Another premise for the work is that capacity considerations and associated reliability analysis are omitted in favor of a focus on the uncertainty in the response itself. In order to highlight this point, series and parallel systems are employed as introductory examples. Such systems are implicitly embedded in almost any computational simulation model for actual structures. Instead of redundancy and system effect factors, which are important concepts in capacity considerations, the significant effect of correlation on the response dispersion is here demonstrated.

Among other questions answered in this paper is what it takes to estimate the mean response in one computational simulation analysis. Inputting mean values for the intervening parameters does not produce the mean response, due to the aforementioned nonlinearities. This paper shows how far off the mean response can be, and by how much the use of first-order and full/limited second-order response sensitivities can improve the estimate.

Keywords:

Uncertainty quantification; Correlation; Finite element analysis; Direct differentiation method.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

On the multi-scale modeling of polymer aging: a microscopic point of view

Giacomo Buccella[1,*], Andrea Villa[2], Luca Barbieri[3], Daniele Palladini[4], Giovanni d'Avanzo[5], Simone Venturini[6]

[1]Research Energy System - RSE, Via Rubattino 54, Milan, Italy, E-mail: giacomo.buccella@rse-web.it [2]Research Energy System - RSE, Via Rubattino 54, Milan, Italy, E-mail: andrea.villa@rse-web.it [3]Research Energy System - RSE, Via Rubattino 54, Milan, Italy, E-mail: luca.barbieri@rse-web.it [4]Research Energy System - RSE, Via Rubattino 54, Milan, Italy, E-mail: daniele.palladini@rse-web.it [5]Research Energy System - RSE, Via Rubattino 54, Milan, Italy, E-mail: giovanni.davanzo@rse-web.it [6]Research Energy System - RSE, Via Rubattino 54, Milan, Italy, E-mail: simone.venturini@rse-web.it

Abstract: We present a multi-scale approach to model the aging of polymeric insulators employed in the electrical power industry. We deal with the degradation derived from partial discharges (PDs), that is, small local discharge events triggered by the electric field inside some gaseous cavities embedded in the material. Our approach is deterministic and based on first principles. It includes the modeling of both microscopic phenomena, such as chemical reactions and electronic drift, and macroscopic phenomena, such as the frequency of PDs.

Polymeric materials used as insulators in the electrical industry undergo wear and aging due to PDs [1, 2, 3], which are responsible for the formation of a plasma inside internal

defects and cavities. The aging of the polymeric insulation is caused by the interaction between the plasma and the solid phase. Examples of aging phenomena include the chemical evolution of the gas/solid interface, surface sputtering or an increase of surface electrical conductivity. In some cases, PDs can sustain the propagation of the defect in the matrix, forming a series of channels. This is known as the treeing effect [4, 5]. The model we are presenting takes into account all these processes, which occur at different physical and temporal scales.

We model several microscopic phenomena that play a key role in the deterioration process of polyethylene (PE), which is vastly employed as dielectric material in high-voltage cables. In particular, we perform first- principles calculations to model some chemical processes involved in treeing. Afterwards, quantum chemistry results are employed to estimate some parameters needed to obtain larger scale modeling [6], comparable with experimental references.

The present work discusses the estimation of some microscopic parameters derived from atomistic modeling and later implemented in larger macroscopic simulations. We investigate the conditions associated with the triggering of each PD taking place within a defect and sustaining treeing propagation. PDs are triggered by an electron emission from a PE surface into the gas (first electron availability). The Schottky effect is believed to be the most likely mechanism able to produce this first emission [7, 8, 9]. The Schottky effect is strongly linked to the work function, thus with a surface's chemical and electronic features. Our calculations suggest that Schottky emission from PE can take place if an excess of electronic charge accumulates on the surface in the presence of a specific chemical defect. However, the estimation of the exact work function is highly uncertain, since it largely depends on the local physico-chemical conditions. By means of molecular

dynamics, we model the interactions between a PE surface and a series of plasma ions. According to our calculations, the most frequent chemical process is the abstraction of a hydrogen atom followed rapidly by the oxidation of the surface [10]. At low energies, the activity of plasma ions is negligible, since they are far fewer than the neutral species. With more intense electric fields and higher-energy impacts, the surface sputtering performed by plasma ions becomes an important phenomenon.

Surface sputtering produces a great number of carbonic fragments to be released in the gas. We model the chemisorption of such carbonic fragments on PE that can lead to the formation of a new chemical phase with increased conductive properties, as discussed in the literature [11, 12]. Such a process results in enhanced charge carrier mobility on the surface, as suggested by our electronic structure modeling.

In the future, we aim to improve the model with more refined descriptions, obtaining chemical data associated with more complex materials. Possible future applications will allow us to predict the remaining lifetime of electrical devices such as high-voltage cables or dry transformers.

Keywords: Multi-scale modeling; Molecular dynamics; Quantum chemistry; Partial discharges

---

* Presenting author

References

[1] T. Farr, R. Vogelsang, and K. Frohlich. A new deterministic model for tree growth in polymers with barriers. In *2001 Annual Report Conference on Electrical Insulation and Dielectric Phenomena*, 2001.

[2] L. Barbieri, A. Villa, and R. Malgesini. A step forward in the characterization of the partial discharge phenomenon and the degradation of insulating materials through nonlinear analysis of time series. *IEEE Electrical Insulation Magazine*, 28(4), 2012.

[3] S. Rowland, R. Schurch, M. Pattouras, and Q. Li. Application of FEA to image-based models of electrical trees with uniform conductivity. *IEEE Transactions on Dielectrics and Electrical Insulation*, 22(3):1537–1546, 2015.

[4] H. Hirose. More accurate breakdown voltage estimation for the new step-up test method in the gumbel distribution model. *European Journal of Operational Research*, 177(1):406–419, 2007.

[5] Y. Sun, S. A. Boggs, and R. Ramprasad. The intrinsic electrical breakdown strength of insulators from first principles. *Applied Physics Letters*, 101(13):132906, September 2012.

[6] A. Villa, L. Barbieri, M. Gondola, A. R. Leon-Garzon, and R. Malgesini. A PDE-based partial discharge simulator. *Journal of Computational Physics*, 345:687–705, 2017.

[7] G. C. Montanari, M. Conti, F. Ciani, A. Cavallini, G. Mazzanti, and S. Serra. First electron availability and PD generation in insulation cavities. In *2003 Annual Report Conference on Electrical Insulation and Dielectric Phenomena*, 2003.

[8] A. Cavallini, F. Ciani, G. Mazzanti, and G. C. Montanari. First electron availability and partial discharge generation in insulation cavities: effect of light irradiation. *IEEE Transactions on Dielectrics and Electrical Insulation*, 12(2):387–394, 2005.

[9] A. Villa, A. R. Leon-Garzon, L. Barbieri, and R. Malgesini. Ignition of discharges in macroscopic isolated voids and first electron availability. *Journal of Applied Physics*, 125:043302, 2019.

[10] A. R. Leon-Garzon, G. Dotelli, M. Tommasini, C. L. Bianchi, C. Pirola, A. Villa, A. Lucotti, B. Sacchi, and L. Barbieri. Experimental characterization of polymer surfaces subject to corona discharges in controlled atmospheres. *Polymers*, 11(10):1646, 2019.

[11] A. S. Vaughan, I. L. Hosier, S. J. Dodd, and S. J. Sutton. On the structure and chemistry of electrical trees in polyethylene. *Journal of Physics D: Applied Physics*, 39(5):962, 2006.

[12] X. Chen, Y. Xu, X. Cao, S. J. Dodd, and L. A. Dissado. Effect of tree and channel conductivity and on electrical and tree and shape and breakdown and in XLPE and cable insulation and samples. *IEEE Transactions on Dielectrics and Electrical Insulation Vol. 18, No. 3; June*, 18(3):847–860, 2011.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Numerical Simulation of Physico-Chemical Systems

Emmanuel Adoliwine Amikiya[1,*], Mapundi K. Banda

[1]Ghana Institute of Management and Public Administration, E-mail: eamikiya@gimpa.edu.gh

[2]University of Pretoria, E-mail: mapundi.banda@up.ac.za

Abstract: Mathematical models for chemical reactions that occur simultaneously with transport processes such as advection and diffusion (physico-chemical systems), are characteristically nonlinear and challenging to simulate due to stiffness, high degrees of freedom and spatial heterogeneity. While stiffness constrain some numerical schemes, high degrees of freedom and spatial heterogeneity increase cost of simulation. Model re-duction methods can reduce the degrees of freedom, however, not all numerical methods are compatible with model reduction methods. Therefore, the challenge is to design simulation procedures that can simultane- ously resolve stiffness, nonlinearity and are compatible with model reduction methods. Such procedures are rare in the literature. In this work, we discuss numerical simulation procedures that can resolve stiffness, significantly reduce the high degrees of freedom, resolve nonlinearity and reduce high cost of simulation. Simulation experiments have been conducted to establish the efficiency and suitability of the procedures for reactive transport processes.

Keywords: Physico-chemical systems, Nonlinear models, Numerical simulation, Model reduction and Sto- ichiometric method.

* Presenting author

References

[1] Petzold L. and Zhu W., Model Reduction for Chemical Kinetics: An Optimization Approach, AIChE Journal 45(4) (1999) 869-889.

[2] Zhuyin R. and Stephen B. P., Second-order splitting schemes for a class of reactive systems, Journal of Computational Physics 227 (2008) 8165-8176.

[3] Walton S., Hassan O., and Morgan k., Reduced order modelling for unsteady fluid flow using proper orthogonal decomposition and radial basis functions, Applied Mathemat- ical Modelling 37 (2013) 8930-8945.

[4] Bellen A., Jackiewicz Z. and Zennaro M., Contractivity of waveform relaxation Runge-Kutta iterations and related limit methods for dissipative systems in the maximum norm, SIAM J. NUMER. ANAL. Vol. 31, No. 2, (1994) pp. 499-523

[5] Ya-Jing H. and Wen-An Y., Partial equilibrium approximations in apoptosis I. The intracellular-signalling subsystem, Mathematical Biosciences, 2013, 246, 27–37.

[6] Ya-Jing H. and Wen-An Y., Partial equilibrium approximations in apoptosis II. The death-inducing signalling complex subsystems, Mathematical Biosciences, 2013, 246, 27–37.

[7] Goussis D. A., Quasi steady state and partial equilibrium approximations: their relation and their validity, Combustion Theory Model, 2012, 16 (5), 86–926.

[8] Fricker N., Beaudouin J., Richter P., Eils R., Krammer P.H., and Lavrik I.N., Model- based dissection of CD95 signaling dynamics reveals both a pro-and antiapoptotic role of c-FLIPL, Journal Cell Biology, 190 (3), 2010, 377–389.

[9] S. Lam, D. Goussis, Understanding complex chemical kinetics with computational singular perturbation, in: Proceedings of International Symposium on Combustion, 22, Elsevier, 1989, 931–941.

[10] Huang Y. J., and Yong W. A., A stable simplification of a Fas-signaling pathway model for apoptosis, in: Proceedings of the 2012 IEEE 6th International Conference on Systems Biology (ISB), IEEE, 2012, 12–134.

[11] Keener J.P., and Sneyd J., Mathematical Physiology, Springer, 1998.

[12] Djouad R. and Sportisse B., Solving reduced models in air pollution modelling, Applied Numerical Mathematics, 2003, 49–61.

[13] Amikiya A.E. and Mapundi B., A stoichiometric method for reducing simula- tion cost of chemical kinetic models, Computers & Chemical Engineering 112 https://doi.org/10.1016/j.compchemeng.2018.02.020

[14] Blom J.G., and Verwer J.G., A comparison of integration methods for atmospheric transport-chemistry problems, Journal of Computational and Applied Mathematics 126 (2000) 381-396.

[15] Verwer J.G., Sommeijer B.P., Hundsdorfer W., RKC time-stepping for advection-diffusion-reaction problems, Journal of Computational Physics 201 (2004) 61-79.

[16]David L. R., John N. S., and Curtis C. O, Studies of the accuracy of time integration methods for reaction-diffusion equations, Journal of Computational Physics 194 (2004) 544-574.

[17]Anne B., Anita T. L., and Michael L. M., High-order multi-implicit spectral deferred correction methods for problems of reactive flow, Journal of Computational Physics 189 (2003) 651-675.

[18] Yulong X. and Shu C., High-order finite volume WENO schemes for the shallow water equations with dry states, Advances in Water Resources 34 (2011) 1026-1038.

[19]Werner S. and Lee F. G., Oxygenation of ferrous iron, American Chemical Society,1961, 53, 143–146.

[20] Ayora C., Manuel A. C., Francisco M., Tobias S. R., Jesus C. and Jose-Miguel N., Acid mine drainage in the Iberian Pyrite Belt: 2. Lessons learned from recent passive remediation experiences, Environ Sci Pollut Res, 2013, DOI 10.1007/s11356-013-1479-2

[21]Plummer L. N. and Wigley T. M. and Parkhurst D. L., The kinetics of calcite dissolution in CO_2 – water systems at 5^oC to 60^oC and 0.0 to 1.0 atm CO_2, American Journal of Science, 1978, 278, 179–216.

[22] Reddy M. M. and Plummer L. N. and Busenberg E., Crystal growth of calcite from calcium bicarbonate solution at constant P_{CO_2} and 25^oC: a test of calcite dissolution model,Geochimica et Cosmochimica, 1981,45, 1281–1289.

[23] Tian J. and Yong-Tao Z., Krylov implicit integration factor WENO methods for semilin- ear and fully nonlinear advection-diffusion-reaction equations, Journal of Computational Physics 253 (2013) 368-388.

[24] Beylkin G., Keiser J.M. and Vozovoi L., A new class of time discretization schemes for the solution of nonlinear PDEs, Journal of Computational Physics, 147 (1998) 362-387.

[25] Cox S.M., Matthews P.C., Exponential time differencing for stiff systems, Journal of Computational Physics, 176 (2002) 430-455.

[26] Maday Y. , Patera A.T. and Ronquist E.M., An operator-integration-factor splitting method for time-dependent problems: Application to incompressible fluid flow, Journal of Scientific Computing 5 (1990) 263-292.

[27] Kassam A. K. and Trefethen L. N., Fourth-order time stepping for stiff PDEs, SIAM Jorunal Scientific Computing 26(4) (2005) 1214-1233.

[28] Qing N., Yong-Tao Z. and Rui Z., Efficient semi-implicit schemes for stiff systems, Journal of Computational Physics 214 (2006) 521-537.

[29] Willem Hundsdorfer and Jan Verwer, "Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations", Springer-Verlag Berlin Heidelberg, New York, (2003), ISBN 978-3-642-05707-6.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Two Time Scales Modelling of the Irreversible Deformation and Damage Accumulation in Metals and Metamaterials

Dmytro Breslavsky[1,a], Oksana Tatarinova[1], Holm Altenbach[2], Francesco Pellicano[3]

[1]National Technical University 'Kharkiv Polytechnic Institute',

E-mail: Dmytro.Breslavsky@khpi.edu.ua, Oksana.Tatarinova@khpi.edu.ua

[2]Otto von Guericke University, Magdeburg, E-mail: holm.altenbach@ovgu.de

[3]University of Modena and Reggio Emilia, E-mail: francesco.pellicano@unimore.it

Operating modes with cyclic varying of loads and irreversible deformation of the material often arise in practical applications. Direct numerical modeling of such processes, for example, creep or low-cycle fatigue, requires significant computational resources and in many cases cannot be carried out due to the accumulation of computational errors. The use of the method of many scales and averaging over the period of cyclic stress varying is an effective way to solve such problems.

The problems of deformation and damage accumulation at cyclic loading are considered. A general three-dimensional initial-boundary value problem of irreversible deformation under cyclic loading with high (forced oscillations) or low frequencies (low-cycle deformation) is posed [1]. By expanding the main unknowns (displacements, strains, stresses) in a series with a small parameter followed by averaging over the period of cyclic varying, two related systems of equations are obtained. In a similar way, averaged equations of state and damage evolution equations are developed. A comparison of experimental and numerical data obtained using the proposed constitutive equations is analyzed.

The formulated averaged problems are solved by the Finite Element method using time- difference integration schemes. The developed Finite Element modeling tools for general 3D and 2D stress states are discussed.

As examples, the problems of high-temperature high- and low-cycle deformation, accompanied by the accumulation of hidden damage, are considered. The results of modeling the creep of titanium alloy plates under tension and high-frequency bending are discussed. The obtained data are compared with experimental ones. The data of the analysis of low-cycle high- temperature deformation and the accumulation of damage in a shell made of bronze are presented. The results of the calculation of static and cyclic creep during bending of a metamaterial plate, which is a three-layer structure with two thin outer plates and an auxetic inner core, are presented.

Keywords: two time scales, cyclic loading, averaging over the period, deformation, creep, damage, metal, metamaterial.

---

[a] Presenting Author

References:

[1] D.Breslavsky, O.Morachkovsky, O.Tatarinova. 2014. Creep and damage in shells of revolution under cyclic loading and heating. International Journal of Nonlinear Mechanics. Vol. 66, pp. 87-95

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Enhancing Computational Efficiency in Probabilistic Wildfire Risk Assessment through a Novel Cluster-Based Active-Learning Methodology

Vishnupriya Jonnalagadda [1] , Ji Yun Lee [2,a]

[1] Washington State University, E-mail: v.jonnalagadda@wsu.edu

[2] Washington State University, E-mail: jiyun.lee@wsu.edu

Over the past four decades, wildfires have become an increasingly serious threat to infrastructure systems and communities, particularly in regions experiencing climate change and increased development in the wildland-urban interface (WUI) [1]. In wildfire-devasted regions, the losses have been staggering. The 2018 California wildfires resulted in 103 deaths and direct economic losses of $26.5 billion, with total costs (including supply chain disruption, lost timber and livelihoods, fire suppression efforts, and post-fire recovery) estimated at $400 billion [2]. Understanding and managing this risk requires a move beyond deterministic assessments and towards a probabilistic approach. Probabilistic wildfire risk assessment provides a more comprehensive picture of potential impacts by explicitly reflecting uncertainties in wildfire ignition, behavior, spread, and containment. However, this approach often relies on computationally expensive simulations, requiring a large number of runs (i.e., possible wildfire scenarios) to accurately characterize the risk. This computational burden can hinder the practical application of probabilistic wildfire risk assessment, especially for large- scale infrastructure systems and communities. Therefore, there is a pressing need for efficient methods to reduce the computational cost while maintaining the accuracy and representativeness of the risk assessment.

To address the computational challenges associated with probabilistic wildfire risk assessment, this study proposes a novel scenario reduction methodology. By strategically selecting a representative subset of wildfire scenarios, the proposed methodology can capture the variability across all potential scenarios without requiring the full set of simulations. The primary goal is to ensure the wildfire hazard curve derived from this subset closely matches that from the full set. This necessitates an optimization problem during the scenario reduction process to minimize the discrepancy between the two hazard curves. Our strategy focuses on achieving accuracy not only for the entire study area but also for individual cells within the area.

We develop this methodology based on the principle of active learning by addressing several limitations: (1) a random initial training set that can slow the learning process, (2) an inability to focus on both macro and micro scales, and (3) a lack of event probability assignment. To address these shortcomings, our methodology integrates the unsupervised learning technique of clustering (e.g., k-means clustering) with supervised active learning (see Fig. 1). Here, active learning will be guided and enhanced by clustering techniques, making the sampling process more efficient and effective. As shown in Fig. 1(a), we first represent all wildfire scenarios generated from our in-house simulation model as data points in an N- dimensional space, where N is the total number of spatial units within the study area. Each axis represents a specific spatial unit's burnt extent (or other fire consequence measures). Then, we will choose initial centers for k clusters, assign scenarios to each cluster, and update the cluster centers [3]. These cluster centers serve as the initial reduced set of wildfire scenarios. As such,

the clustering process can organize or segment wildfire scenarios into clusters based on their potential consequences to the study area.

In the active learning process, to maximize learning effectiveness, we sequentially add data points based on their impact on the discrepancies between true and estimated hazard curves until a predefined stopping criterion is met. Once a final reduced set is determined, we return to the clustering algorithm, setting the data points in the final subset as new cluster centers. Finally, the remaining data points are reassigned to these cluster centers, and the probabilities of the wildfire scenarios in this final subset are calculated. In summary, the proposed methodology will identify diverse, representative samples from different regions of the data space and assign probabilities via clustering, while enhancing accuracy at both macro and micro levels. By providing a more complete picture of wildfire risk, this methodology will empower communities and policymakers to make informed decisions that ultimately reduce the consequences of wildfire events, safeguarding lives, property, and essential services.

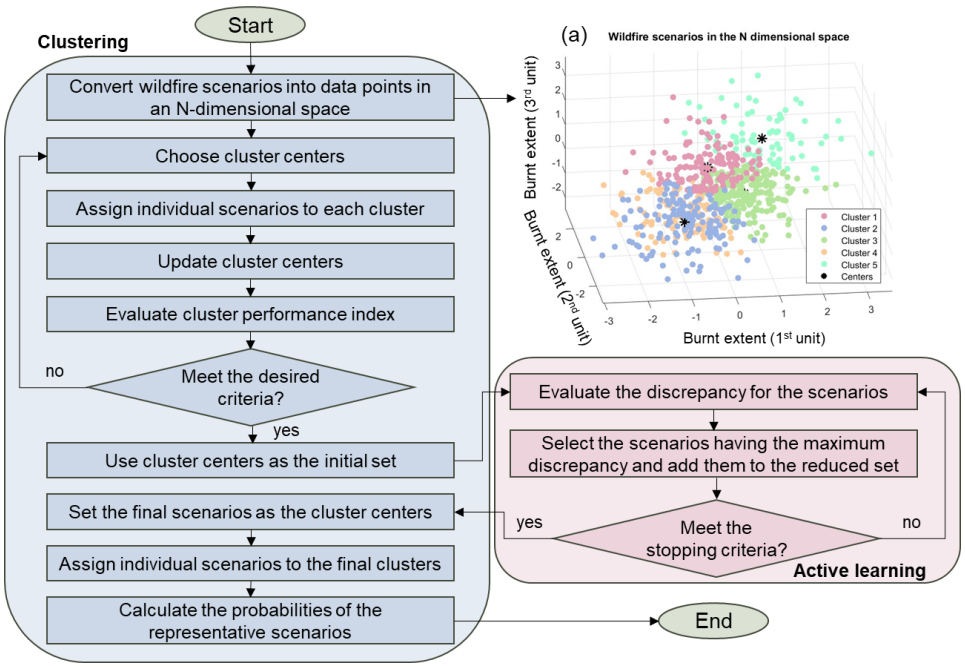


Figure 1. A procedure for the proposed clustering-based active learning methodology

Keywords: Wildfires; Risk assessment; Probabilistic approach; Clustering; Active learning; Machine learning; Simulation; Scenario

---

[a] Presenting Author

References:

[1] J. S. Fried, M. S. Torn, & E. Mills. 2004. The impact of climate change on wildfire severity: a regional forecast for northern California. *Climatic change*, 64(1), pp. 169-191.

[2] J. Roach. 2019 Nov. California wildfires will cost tens of billions. *AccuWeather*.

[3] S. Lv, J. Li, Y. Guo, & Z. Shi. 2019. A typical distributed generation scenario reduction method based on an improved clustering algorithm. Appl. Sci., 9(20), pp. 9-23.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

GReS: A novel multi-physics multi-domain computational tool for geomechanical subsurface simulations

Massimiliano Ferronato [1,a], Andrea Franceschini[2], Daniele Moretto[3]

[1] University of Padova, Italy, E-mail: massimiliano.ferronato@unipd.it

[2] University of Padova, Italy, E-mail: andrea.franceschini@unipd.it

[3] University of Padova, Italy, E-mail: daniele.moretto.3@phd.unipd.it

It is very well-known that the prediction of the geomechanics plays a crucial role for a proper management of underground resources, involving multiple physical processes, such as fluid flow, poromechanics, fault activation, thermal flow, and chemical reactions, that can take place simultaneously with multiple time and space scales. Despite a lot of work has been already done for the analysis and simulation of individual subsurface processes, research is still very active in the attempt of coupling geomechanics with other relevant phenomena at the proper scale, from both a numerical and a physical point of view.

GReS is a novel open-source modular platform, specifically designed with the aim at contributing to the development and prototyping of numerical algorithms for fully coupled multi-physics multi-domain geomechanical applications. The idea is to partition the overall computational domain into possibly non-conforming subdomains where different physics and discretization schemes can be used. The

code is based on a high-level programming platform (MATLAB) that should lower the entry barrier for new users and developers, as well as the effort for implementing and testing innovative numerical algorithms. Moreover, the modular structure of the code encourages contributions from different developers at variable levels, from the implementation of new physics and discretization schemes to specific algorithms to accelerate the linear and non-linear solver. Despite being primarily conceived as a prototyping platform, GReS wraps low-level advanced linear algebra packages to combine simplicity with fair efficiency.

In the present communication, we will introduce the GReS concept and its current development state, including advances to the mortar algorithm used to transfer the information among non-conforming subdomains with independent meshes. Basic benchmarks will be presented to show the current code's potentials, along with the projects for future developments.

Keywords: coupled poromechanics, multi-domain simulations, mortar method

[a] Presenting Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Modeling of Metal Matrix Composites considering phase debonding and porosity using FEM and the RVE concept

JOSE J. C. PITUBA [1,a], GEOVANA A. RIBEIRO [2], WANDERSON F. SANTOS [3], GABRIELA R. FERNANDES [4]

[1] Federal University of Catalão (UFCAT), E-mail: julio_pituba@ufcat.edu.br

[2] Federal University of Catalão (UFCAT), E-mail: geovanaalves@discente.ufcat.edu.br

[3] University of Sao paulo (USP), E-mail: wanderson_santos@usp.br

[4] Federal University of Catalão (UFCAT), E-mail: gabrielar.fernandes@ufcat.edu.br

Porous materials can be obtained in different situations. In some cases, voids are introduced to the material to obtain specific properties, for example, a lighter material. However, the voids can also be resulted from defects in the material, which occur during the fabrication process or after loading, [1]. In the present work, we studied the case of metallic materials reinforced by rigid inclusions whose microstructure contains voids, called metal matrix composites (MMC). This kind of material has different applications. To model the mechanical behavior of MMC, a Finite Element Method (FEM) formulation based on Representative Volume Element (RVE) concept is used considering the plasticity phenomena as well as phase debonding when occurs on the interfacial transition zone (ITZ) [1].

We adopt the matrix as an ideally plastic material governed by the von Mises model with isotropic hardening while inclusions are adopted as very stiff elastic materials. Also, fracture and contact finite elements are used to model the phase debonding [2]. Besides, we consider inclusions perfectly bonded to the matrix in

other analysis to investigate the influence of this assumption. Different distributions of voids and inclusions are assumed.

The formulation is based on the following principles [2]: (1) RVE equilibrium; (2) the Hill Mandel Macrohomogeneity Principle; (3) Volume average of the strain and stress tensors; and (4) the definition of the minimally constrained vector space of kinematically admissible displacement fluctuation of the RVE agrees with the proposition of the volume average of the strain vector. In summary, the solution of the equilibrium problem is found using an iterative procedure, where at each iteration correction for the displacement fluctuation field is computed. After achieving the RVE equilibrium, its homogenized response is computed.

---

[a] Presenting Author

References:

[1] J.J.C. Pituba, W.F. dos Santos, G.A. Ribeiro, G.R. Fernandes. 2021. Computational homogenisation approach applied to improve mechanical properties of heterogeneous materials. Computational and Applied Mathematics. Vol. 40, n. 187.

[2] J. J. C. Pituba., G. R. Fernandes, E. A. Souza Neto. 2016. Modeling of Cohesive Fracture and Plasticity Processes in Composite Microstructures. Journal of Engineering Mechanics. Vol. 142, 04016069.

.

We Applied the RVE based formulation [2] to perform numerical analyses in microstructures reinforced by different volume fraction of inclusions (vf =2.5%, vf = 5%, vf

= 7.5%, vf =10% and vf =12.5%) with and without porosity. When the porosity is considered, its values are adopted equal to the volume fraction of inclusion. We verified that the RVE with 2.5% of volume fraction of inclusion and without porosity, has presented the best structural behavior. However, among the RVEs with porosity, the one with vf = 2.5% has presented the best performance. Bigger values of volume fraction of voids and inclusion significantly reduce the RVE loading capacity and, in several cases, lead to failure of the material. Thus, the porosity and the addition of a very stiff elastic inclusion must be controlled to not worsen the material properties. In this case, this control can be difficult, and it is better to consider porous metallic material without reinforcement to have a material with better properties.

Keywords: metal matrix composites; RVE; plasticity; cohesive fracture.

Acknowledgements: This work was financially supported by CNPq (National Council for Scientific and Technological Development) [grant numbers 305927/2023-0 and 303863/2023-4]

Liquid Phase behavior and Molecular aggregation in Aqueous Solutiyons: MD Simulation and Graph Theoretical Analysis

Ravi Singh[1] and Jun-Ho Choi [1,a]

[1] Department of Chemistry, Gwangju Institute of Science and Technology (GIST), Republic of Korea,

Email: junhochoi@gist.ac.kr

Recently, some computational attempts to describe the phase behavior in binary aqueous mixtures in terms of molecular aggregation were made. [1] Combination studies of MD simulation and graph theoretical analysis enable it to propose distinct aggregation pathway, caused by intermolecular interaction between water and solute molecules. That is, self- associated aggregates are formed by avoiding interaction with water, while significant interaction of water-solute facilitates formation of spatially extended aggregates. It was shown that the spatial distribution of component molecules is determined by distinct aggregate pattern in the binary liquid mixtures. [2] Formation of self-associated aggregates cause spatial inhomogeneity, whereas uniform distribution of constituent molecules in given mixtures is accompanied by existence of spatially extended aggregates.

Based upon MD simulation and graph theory in given molecular systems, the molecular aggregation behavior and water H-bond network properties were examined in n-butanol-water and triethylamine (TEA)-water mixtures, which exhibit upper critical solution temperature (UCST) [3] and lower critical solution temperature (LCST) type [4], respectively. It is addressed how temperature affects aggregation behavior of solute molecules and network properties of solute and water aggregates, and how distinct aggregation pattern determines the spatial

distribution of component molecules and eventually phase behavior of binary liquid mixtures.

Keywords: molecular dynamics (MD) simulation, graph theory, binary liquid mixture, water H-bond network, spatial inhomogeneity, molecular aggregation

---

[a] Presenting Author

References:

[1] S. Choi, S. Parameswaran and J.-H. Choi. 2020. Understanding Alcohol Aggregates and Water Hydrogen Bond Network Towards Miscibility in Alcohol Solutions: Graph Theoretical Analysis. Phys. Chem. Chem. Phys. Vol. 22, pp. 17181-17195.

[2] J. Seo, S. Choi, R. Singh and J.-H. Choi. 2023. Spatial Inhomogeneity and Molecular Aggregation behavior in Aqueous Binary Liquid Mixtures. J. Mol. Liq. Vol. 369, p. 120949.

[3] S. Parameswaran, S. Choi and J.-H. Choi. 2022. Temperature Effects on Alcohol Aggregation Phenomena and Phase Behavior in n-butanol Aqueous Solution. J. Mol.Liq. Vol. 347, p. 118339.

[4] R. Singh, J. Seo, J. Ryu and J.-H. Choi. 2024. Unraveling the interplay of temperature with molecular aggregation and miscibility in TEA–water mixtures. Phys. Chem. Chem. Phys. Vol. 26, pp. 18970-18982.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Concrete in Nuclear Shielding Applications: A Multi-physics Numerical Study

Jiangkun Zhang [1,a], Beatrice Pomaro [1] and Gianluca Mazzucco [1]

[1] Department of Civil, Environmental and Architectural Engineering (DICEA) University of Padova (UNIPD)

Via F. Marzolo 9, 35131 Padova, Italy.

E-mail: jiangkun.zhang@unipd.it, beatrice.pomaro@unipd.it, gianluca.mazzucco@unipd.it

Nuclear power is increasingly recognized as a critical solution to mitigate the global energy crisis. Among the essential components in nuclear power plant design, the concrete biological shield serves as a crucial barrier to prevent nuclear radiation leakage during operation. However, over long-term operation the structural integrity of this shield deteriorates due to the combined effects of mechanical loads, radiation, temperature fluctuations, and change in moisture content. Predicting the behaviour of irradiated shielding concrete requires advanced multi-physics coupled numerical models that comprehensively address these interactions.

Current challenges in modelling numerically concrete behaviour in nuclear environments mainly include: i. realistic mesoscale representations of concrete in terms of grading curve, aggregate content, and geometric heterogeneity; ii. accurate distribution of neutron fluxes, and iii. incorporation of the confinement effects exerted by aggregates and reinforcement on the cement paste. In this study, these aspects are all considered in simulating an experimental campaign from the literature [1]. Specifically, the numerical analyses are conducted at the

mesoscale, on solid sample models characterized by different grading curves and aggregate contents. These samples are generated using a random distribution algorithm [2] in compliance with the provided target mix design. The damage evolution within the irradiated concrete samples is studied with a Finite Element fully coupled thermo-mechanical and neutron diffusion model [3].

Simulation results span irradiation periods from 25 to 300 days under varying confinement conditions. The decay of the Young's modulus and the compressive strength of the irradiated samples is derived numerically through the stress-strain curves obtained simulating uniaxial compressive experiments after different irradiation times. The evolution of

---

[a] Presenting Author

References:

[1] I. Maruyama, O. Kontani, M. Takizawa, S. Sawada, S. Ishikawao, J. Yasukouchi, O. Sato,

J. Etoh, and T. Igari. 2017. Development of soundness assessment procedure for concrete members affected by neutron and gamma-ray irradiation. Journal of Advanced Concrete Technology, Vol. 15, pp. 440–523.

[2] G. Mazzucco, B. Pomaro, V. A. Salomoni, and C. E. Majorana. 2024. Three-dimensional meso-scale modeling of asphalt concrete. Computers & Structures, Vol. 305, pp. 107535.

[3] J. Zhang, B. Pomaro, G. Mazzucco, B. F. Dongmo, C. Majorana, and V. Salomoni. 2024. A 3D coupled thermo-mechanical and neutron diffusion numerical model for irradiated concrete. International Journal of Mechanical Sciences, Vol. 264, pp. 108806.

the two key mechanical properties with irradiation times are found in good agreement with reported experimental data, confirming the model's accuracy.

Significant findings of the present study include: i. Radiation-induced volume expansion on aggregates initiates observable damage in concrete after 100 days of irradiation, for the specific operational scenario. ii. The aggregate type substantially influences damage evolution. iii. The incorporation of the effects of confinement on the cement paste significantly affects the stress distribution on concrete locally. In conclusion, this research provides a robust framework for assessing the long-term performance of nuclear biological shields, towards a comprehensive study of durability of nuclear infrastructures.

Keywords: Nuclear biological shield; Irradiated concrete; Mesoscale modelling; Thermo- mechanical coupling; Radiation-induced damage.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Multiple time-weighted residual methodology for the design of linear multi-step time integration algorithms

Yazhou Wang1,*, Nikolaus Adams2, Kumar Tamma3 [1]Technical University of Munich, E-mail: yazhou.wang@tum.de

[2]Technical University of Munich, E-mail: nikolaus.adams@tum.de

[3]University of Minnesota–Twin Cities, E-mail: ktamma@umn.edu

Abstract: The design of time integration algorithms is a fundamental challenge in advancing modern computational platforms, particularly for time-dependent simulations in structural dynamics across scientific simulations on science and engineering disciplines. Dating back to the Houbolt method developed in the year 1950, numerous Linear Multi-Step (LMS) methods have been developed via a certain mathematical basis, such as the finite difference approximation, Taylor-series expansion, time-weighted residual approach, manufactured formulation, and so on. Among these approaches, the time-weighted residual approach has proven to be particularly powerful. It has been utilized in the design of first-generation Generalized Single- Step Single-Solve (GS4) computational framework [1, 2], encompassing most of the LMS methods which are second-order time accurate as subsets. To date, only the single time-weighted residual approach has been applied mostly since the work of Zienkiewicz [3]. However, since then, Tamma's research group has identified some basic concepts and novel ideas using double weighted time fields to design time integration methods and explain this new idea [2]. These concepts

have opened new possibilities in the design of time integration algorithms but remain underdeveloped.

The primary contribution of this work is the demonstration of a multiple time-weighted residual method- ology, which provides a unified theory to not only explain all the existing efforts on the design of LMS methods in the past 75 years or so, but also lead to new avenues and designs with improved numerical properties over the existing state-of-the-art in certain situations. By leveraging single, double, and triple time-weighted residuals in single, two, and three-field forms of the structural dynamic problem, respectively, we develop a new generation of GS4 algorithms for second-order time-dependent systems. This approach yields the GS4-II$_p$, GS4-II$_{p,q}$, and GS4-II$_{p,q,r}$ computational frameworks, offering analysts a wide bandwidth of design options. The proposed optimal schemes [4] via the multiple time-weighted residual methodology are mainly designed to achieve: second-order time accuracy in all the variables, unconditional stability, zero-order overshooting avoiding the role of initial conditions with/without physical damping, controllable numerical dissipation/dispersion in middle and high frequencies, minimal number of numerical variables (op- timal computational complexity and memory storage), and including certain subsets with truly self-starting property.

In addition, the significant bonus is that you only need to implement a single analysis program for multi- physics problems. The proposed theoretical concepts can all be integrated into a single unified framework and routine, providing a wide choice and varied options to analysts simply by adjusting a few parameters, without having to implement each and every algorithm on a one-by-one basis. This is powerful and noteworthy from the viewpoint of theory development. Moreover, an equally important aspect is that we have developed universal error estimators that are applicable and can provide optimal

estimates for all these methods in a single setting [5]. Furthermore, the unified theory supports the development of isochronous time integration, enabling the simulation of coupled first- and second-order time-dependent systems and individual problems within a single program subroutine [6]. This capability significantly accelerates the advancement and provides a lot of flexibility and a wide choice of algorithms ideally suited for conducting comparative studies on modern computational platforms for multi-physics problems.

Keywords: Time integration; Time-weighted residual; Linear multi-step methods; Generalized single-step single-solve methods

---

* Presenting author

References

[1] X. Zhou, K. K. Tamma. 2006. Algorithms by design with illustrations to solid and structural mechanics/dynamics. International Journal for Numerical Methods in Engineering. Vol. 66, pp. 1738–1790.

[2] K. K. Tamma, X. Zhou, & D. Sha. 2000. The time dimension: a theory towards the evolution, classification, characterization and design of computational algorithms for transient/dynamic applications. Archives of Computational Methods in Engineering. Vol. 7, pp. 67-290.

[3] O. C. Zienkiewicz, W. L. Wood, N. W. Hine, & R. L. Taylor. 1984. A unified set of single step algorithms. Part 1: General formulation and applications. International Journal for Numerical Methods in Engineering. Vol. 20, pp. 1529-1552.

[4] Y. Wang, D. Maxam, N. A. Adams, & K. K. Tamma. 2025. On the novel zero-order overshooting LMS algorithms by design for computational dynamics. Computer Methods in Applied Mechanics and Engineering. Vol. 433, pp. 117522.

[5] Y. Wang, T. Xue, K. K. Tamma, D. Maxam, & G. Qin. 2021. A three-time-level a posteriori error estimator for GS4-2 framework: Adaptive time stepping for second-order transient systems. Computer Methods in Applied Mechanics and Engineering. Vol. 384, pp. 113920.

[6] M. Shimada, S. Masuri, & K. K. Tamma. 2015. A novel design of an isochronous integra- tion [iIntegration] framework for first/second order multidisciplinary transient systems. International Journal for Numerical Methods in Engineering. Vol. 102, pp. 867-891.

Modeling of Concrete Microstrucutre by a BEM Formulation Based on the RVE Concept

Maria Julia Marques Silva[1], Caleb Gomes Pitaluga[2], Gabriela R. Fernandes[3], and JoséJ. C. Pituba[4]

[1,2,3,4]Civil Engineering Department, Federal University of Catalão (UFCAT), Av. Dr. Lamartine Pinto de Avelar, 1120, Setor Universitário- CEP 75700-000 Catalão – GO Brazil,

[1]mariajuliamrq@gmail.com [2]calebpitaluga@gmail.com

[3]gabrielar.fernandes@ufcat.edu.br [4]julio_pituba@ufcat.edu.br

We use a 2D Boundary Element Method (BEM) formulation, based on the representative volume element (RVE) concept, to model numerically the mechanical behaviour of a concrete experimentally tested for compression load (see [1] for details). The BEM formulation used in [1] is developed in details in [2]. This BEM formulation will not be discussed here, for details about it, please see [1], [2] and [3].

To find the microstructure (RVE) that better represents the experimental test, we considered the following quantity of circular aggregates randomly distributed over the RVE domain (see Figs. 1a, 1b, 1c, 1d): 16, 25, 36 and 45 and with the same volume fraction of aggregates adopted in the experimental test which was approximately 40%. Besides, for each RVE we adopted three different diameters for the aggregates, being the bigger diameter not bigger than the value used in the experimental test. For these four RVEs we also considered different modelling for the fracture process at ITZ (Interfacial Transition Zone), by adopting the following regions where this fracture process is modelled: i) around all aggregates, ii) around the medium and big aggregates; iii) only around the bigger aggregates.

The fracture process at ITZ is modelled by defining cohesive-contact finite elements on the interfaces (for more details about these elements and for the parameters values used in their fracture and contact models, see [1], [2] and [4]). The number of cells, boundary elements, interface elements and of cohesive-contact elements are, respectively, for RVE 16, RVE 25, RVE 36 and RVE 45: 598, 68, 180 and 108: 634, 68, 220 and 60; 982, 80, 344 and 60; 1224, 92, 424 and

128. These discretizations are referred to the case where the fracture process is modelled only around the bigger aggregates. For the matrix we adopted: Young's modulus (EM) = 23Gpa; Possion's ration (νM) = 0.2, the Mohr-Coulomb criterion with Friction Angle (ϕ) = 4° and plasticity curve (effective plastic strain, yield stress) defined by the points: (0;11MPa) (0.22;40MPa). We

adopted elastic aggregates with the properties: ν=0.3, E=40GPa. Regarding the quantity and dimensions of circular aggregates for each RVE, RVE 16 has 9 aggregates with 19mm diameter, 4 with 17mm and 3 with 15mm; RVE 25, has 5 aggregates with 19mm diameter, 6 with 15mm and 14 with 12mm; RVE 36 has 5 aggregates with 19mm, 9 with 13mm and 22 with 9mm; RVE 45 has 8 aggregates with 17mm, 12 with 10mm and 25 with 8mm.

We found that the experimental results were satisfactory captured when we considered 25 aggregates and the fracture process modelled only around bigger aggregates (see Fig. 1c). Although, the other numerical responses of the four RVEs were similar (see Fig. 2a), where all results refer to the RVEs where the fracture process is modelled only around bigger aggregates.

Therefore, we concluded that the size and quantity of the aggregates do not have great influence on the concrete mechanical behaviour.

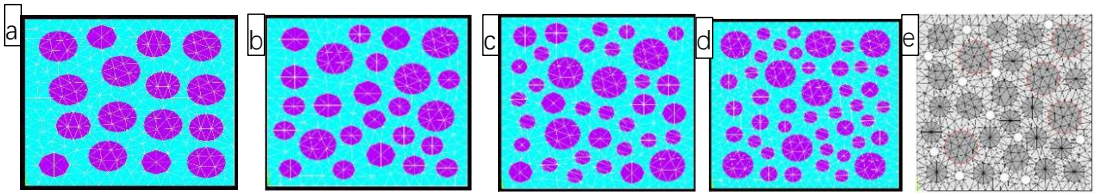


Figure 1– Different distributions of aggregates in the RVE domain **:** (a) RVE 16, (b) RVE 25, (c) RVE 36, (d) RVE 45, (e) RVE-25B with 3.34% of void volume fraction

Then we have inserted 3.34% of porous in the mortar domain of RVE 25B (see fig. 2e), obtaining the RVE-25B-3.34%V. Besides, we increased the isotropic hardening of the mortar matrix to increase the RVE strength, obtaining the RVE-25B-3.34%VF. The points of the plastic curve in RVE-25B-3.34%VF are defined as: (0;11MPa) (0.22;70MPa). We observe in Fig. (2b) that the porosity insertion is very important to better reproduce the concrete behaviour. As final conclusions we can say that the proposed numerical model is efficient, robust, and accurate, as it was capable to reproduce the experimental test.

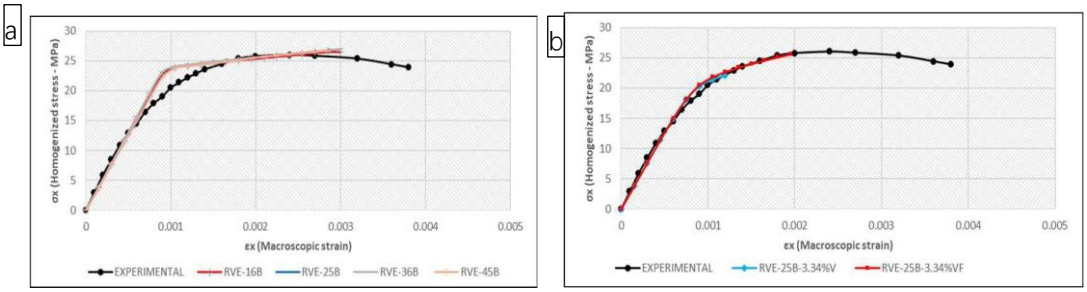


Figure 2-Homogenised stress in the *x* direction, throughout the incremental strain of a) RVE-16B, RVE-25B, RVE-36B, and RVE-45B; b) RVE -25B-3.34%V and RVE -25B-3.34%VF

Keywords: *Boundary elements; zoned plates; homogenisation techniques; RVE; plasticity; cohesive fracture.*

References

[1] M. J. M. Silva; C. G. Pitaluga; G. R. Fernandes; J. J. C. Pituba. Meso-scale modeling of the compressive mechanical behavior of concrete by a RVE-based BEM formulation. *Mechanics of Advanced Materials and Structures.* , v.1, p.1 - 20, 2022.

[2] G. R. Fernandes, M. J. M. Silva, J. F. Vieira, J. J. C. Pituba. A 2D RVE formulation by the boundary element method considering phase debonding. *Engineering Analysis with Boundary Elements*. v.104, p.259 - 276, 2019.

[3] G. R. Fernandes; L. H. R. Crozariol; A. S. Furtado; M. C. Santos. A 2D Boundary Element Formulation to Model the Constitutive Behaviour of Heterogeneous Microstructures Considering Dissipative Phenomena. *Engineering Analysis with Boundary Elements*, v.99, p.1

- 22, 2019.

[4] J. J. C. Pituba.; G. R. Fernandes; E. A. Souza Neto. Modeling of Cohesive Fracture and Plasticity Processes in Composite Microstructures. *Journal of Engineering Mechanics*, v. 142,

p. 04016069, 2016.

Developing Deep Learning Potential for Molecular Dynamics Simulation on Al-Nb-Ti-V-Zr High-Entropy Alloy Hydrogen Storage Materials

An-Zhi Lin[1,a],Shin-Pon Ju[2], Hui-Lung Chen[3], Hsin-Tsung Chen[4]

[1] Department of Mechanical and Electro-Mechanical Engineering, National Sun Yat-sen University, Kaohsiung 80424, Taiwan: d133020001@ nsysu.edu.tw

[2] Department of Mechanical and Electro-Mechanical Engineering, National Sun Yat-sen University, Kaohsiung 80424, Taiwan:jushin-pon@mail.nsysu.edu.tw

[3]Department of Chemistry and Institute of Applied Chemistry, Chinese Culture University, Taipei, 111, Taiwan

[4]Department of Chemistry R&D Center for Membrane Technology and Research Center for Semiconductor Materials and Advanced Optics Chung Yuan Christian University, Chungli District, Taoyuan City 320314, Taiwan

High-entropy alloys (HEAs) are a class of multi-principal element alloys first proposed by Yeh et al. in 2004 [1]. They are defined as single-phase disordered solid solutions composed of five or more metallic elements, with each element's concentration ranging from 5% to 35 at% [1]. Due to their diverse elemental compositions and unique structural effects, HEAs demonstrate advantages such as high hydrogen storage capacity and excellent stability, making them promising candidates for hydrogen storage materials. Montero et al. demonstrated that the addition of 10% Al to the Ti-V-Zr-Nb HEA not only significantly reduces the density of the HEA but also lowers the hydrogen desorption temperature from 270 °C to 160 °C. Furthermore, after multiple adsorption/desorption

cycles, the HEA alloy displayed a reversible gravimetric capacity of around 94% of its initial capacity, outperforming the cycling stability of 85% observed without the Al addition [2].

This study aims to develop a deep learning potential (DLP) that accurately describes the interactions among Al, Nb, Ti, V, Zr, and H elements. First-principles calculations were performed using Density Functional Theory (DFT) [3] to compute the system energy, atomic forces, and virial stress for all structures. These results served as training data for training the DLP using the open-source software DeePMD-kit [4] and DP-GEN [5] with deep neural networks. The differences between the DFT and DLP simulation results were then evaluated to establish a transferable and versatile DLP applicable to the Al-Nb-Ti-V-Zr-H system. A series of Perl scripts [6][7][8][9][10]developed by Ju's group were used to generate the DFT dataset for DLP training and validation systematically.

We categorized and quantified the number of alloy structures used for DFT calculations. These structures were divided into two sources: "Materials Project" and "Self-Generated." The structures from the Materials Project include unary, binary, and ternary alloys, covering BCC, FCC, and HCP crystal types, with quantities of 67, 42, and 10, respectively. The self-generated structures consist of quinary alloys and senary hydrides, also corresponding to BCC, FCC, and HCP crystal types. The quantities for the quinary alloys are 140 (BCC), 204 (FCC), and 140 (HCP), while the senary hydrides exhibit identical quantities. Additionally, the self-generated structures account for the cubic crystal planes (100), (110), and (111), highlighting the diversity and detailed categorization of the designs.

The training and validation performance of the model demonstrates that the Root Mean Square Error (RMSE) gradually decreases with the number of training steps. This trend encompasses training and validation metrics for total energy, forces, and virial stress, indicating consistent improvement in model performance during training. Moreover, the

comparison between predicted and actual values shows that the energy, force, and virial stress prediction plots closely align with the diagonal, reflecting the high accuracy of the predictions.

Finally, the DLP was applied in Molecular Dynamics (MD) simulations to investigate the structural stability under the NPT ensemble at a temperature of 600 K.

Keywords:

High-Entropy Alloy (HEA), Deep Learning Potential (DLP), Molecular Dynamics (MD)

——————————————

References:

[1] Yeh, J-W., et al. "Nanostructured high-entropy alloys with multiple principal elements: novel alloy design concepts and outcomes." Advanced engineering materials 6.5 (2004): 299-303.

[2] Montero, Jorge, et al. "How 10 at% Al addition in the Ti-V-Zr-Nb high-entropy alloy changes hydrogen sorption properties." Molecules 26.9 (2021): 2470.

[3] Verma, Pragya, and Donald G. Truhlar. "Status and challenges of density functional theory." Trends in Chemistry 2.4 (2020): 302-318.

[4] Wang, Han, et al. "DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics." Computer Physics Communications 228 (2018): 178-184.

[5] Zhang, Yuzhi, et al. "DP-GEN: A concurrent learning platform for the generation of reliable deep learning based potential energy models." Computer Physics Communications 253 (2020): 107206.

[6] https://github.com/jushinpon/QE_from_MatCld

[7] https://github.com/jushinpon/make_B2_related_data

[8] https://github.com/jushinpon/make_surface_20240919

[9] https://github.com/jushinpon/dp_train_new

[10] https://github.com/jushinpon/dp_train_label

A Lattice Boltzmann Method for a Range of Flow Regimes: From Free-Flow to Flow in weakly permeable Media

Théo Coiffard[1,*], **Catherine Choquet**[2]

[1]La Rochelle University, E-mail: theo.coiffard(at)univ-lr.fr

[2]La Rochelle University, E-mail: catherine.choquet(at)univ-lr.fr

Abstract: The numerical modelling of flow problems coupling free fluids and porous media is a notoriously difficult problem. If classical continuum-scale models are used, the available approaches suffer from numerous drawbacks. On the one hand, using a Navier-Stokes model in a porous medium is not feasible for large-scale simulations due to the computational cost. On the other hand, if the porous medium is homogenized, it is necessary to couple two systems of partial differential equations with very different structures (Navier- Stokes family and transport equation coupled with a Darcy law) through an interface on which the transfer condition is difficult to calibrate and even non-consensual in the community. The multi-scale nature of this type of problem adds an additional difficulty. For example, to mention only the time scales, the characteristic time of a flow in a coastal aquifer is of the order of kilometers per year, while the characteristic velocities of wave motions in the ocean are of the order of meters per second... And there are numerous examples of applications involving both free and porous media flows: water

management, hydrocarbon exploitation, geological CO_2 and H_2 storage, filtration problems with manufactured materials, modelling of blood flow...

In this presentation, we propose to address this type of problem by disregarding continuum-scale PDE models. We propose a single, purely numerical model that can handle all flow regimes, from free Stokes flow to extremely slow regimes in low-permeability media, within the same computational domain.

To address these challenges, the Lattice Boltzmann Method (LBM) provides a promising alternative. In this class of CFD methods, a fluid density on a lattice is simulated with streaming and collision (relaxation) processes. These basic operations make the numerical scheme highly parallelizable and computationally efficient. As a mesoscopic-scale method, LBM schemes are renowned for their excellent approximation of the Navier-Stokes equations through a judicious choice of the equilibrium distribution function in the collision operator, typically based on the Maxwell-Boltzmann distribution.

Originally designed for free-flow systems, the LBM has been increasingly adapted to address the complexities of porous media. This requires careful consideration of the interactions at the interface and the constraints imposed by the porous structure. Several models (see *e.g.* [5-7]) have been proposed to modify the streaming step in the LBM, which can be expressed as:

$$f_i(x + c_i\Delta t, t + \Delta t) = (1 - \theta)\phi_f f(x, t) + \phi_b b(y, t), \quad (1)$$

$$i \qquad opp(i)$$

where $\theta \in [0, 1]$, ϕ_f corresponds to the phase of the streaming step, and ϕ_b to the reflective distribution phase. When $\theta = 0$, the classical LB scheme is recovered, where ϕ_f is typically

chosen as the post-collision step. When $\theta = 1$, the scheme reduces to the bounce-back rule, allowing the modeling of homogeneous Dirichlet conditions.

Let

$\theta = O(\epsilon^{\alpha}), \quad \epsilon = \Delta x/L, \quad \alpha \geq 0,$

where Δx is the spatial step of the scheme and L a macroscopic length of the domain. For a Multi Relaxation Time model [2] D_2Q_9 model, Chen et al. [1] demonstrated that for $\alpha = 1$, the solution of (1) behaves as the solution of a Darcy-Brinkman model. We extend their results by proving the following asymptotic behaviours:

- For $\alpha = 2$, the scheme also converges to a Darcy-Brinkman model;
- For $\alpha = 3$, it converges to a Stokes model;
- For $\alpha < 1$, the diffusion term becomes negligible for sufficiently large physical lengths, allowing the scheme to approximate Darcy's law.

These theoretical results are validated by several numerical tests for different regimes, ranging from Stokes to Darcy. These tests confirm the consistency and accuracy of the proposed scheme across different flow regimes.CM3P 2025 - Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems

2–4 July 2025, Porto, Portugal

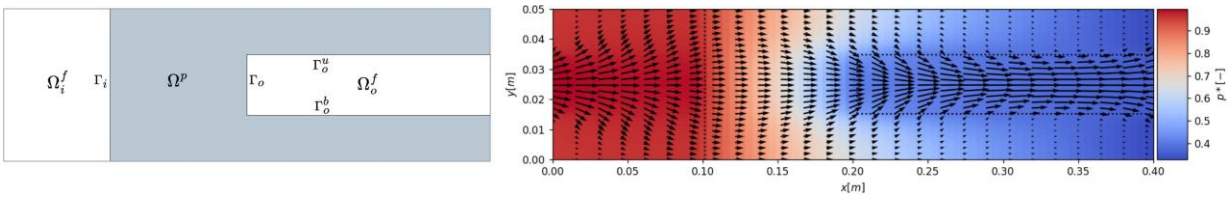


Figure 1: Example of numerical validation: pipe-flow in a soil block (test case inspired of [3]). Geometry (left) and computed velocity and pressure (right)

Further, numerical experiments for domains containing both free parts and porous media are presented. A unique scheme in the form (1) is constructed for the simulations in the whole domain, only θ is tuned in the different subdomains. No special treatment of the interface conditions is required. An illustration is provided in Figure 1.

This study demonstrates the robustness and adaptability of the proposed Lattice Boltzmann Method (LBM) for simulating flows in porous media across different scales. By varying the parameter θ, the model captures transitions from free-flow regions ($\theta = 0$) to porous zones ($\theta = \epsilon^1$ or ϵ^2) and fully solid obstacles ($\theta = 1$), ensuring stability and accuracy in all cases.

Keywords: Porous media - Darcy's law - Darcy-Brinkman model - Stokes flow - Multiscale simulation

---

* Presenting author

References

[1] Chen, C., Li, L., Mei, R., Klausner, J. 2018. Chapman–Enskog Analyses on the Gray Lattice Boltzmann Equation Method for Fluid Flow in Porous Media. *Journal of Statistical Physics*. Vol. 171. DOI: 10.1007/s10955-018-2005-1.

[2] D'Humi`eres, D. 1992. Generalized lattice Boltzmann Equations, Rarefied Gas Dynamics: Theory and Simulations. *Progress in Astronautics and Aeronautics*. Vol. 159, pp. 450–458.

[3] Fujisawa, R., Murakami, Y. 2018. Numerical analysis of preferential flows in soils by the Darcy-Brinkman equations. *Soils and Foundations*. Vol. 58, pp. 1240–1259.

[4] Walsh, S. D. C., Burwinkle, H., Saar, M. O. 2009. A new partial-bounceback lattice-Boltzmann method for fluid flow through heterogeneous media. *Comput. Geosci.* Vol. 35,

pp. 1186–1193.

[5] Yoshida, H., Hayashi, H. 2014. Transmission–Reflection Coefficient in the Lattice Boltzmann Method. *Journal of Statistical Physics*. Vol. 155, pp. 277–299.

[6] Zhu, J., Ma, J. 2013. An improved gray lattice Boltzmann model for simulating fluid flow in multi-scale porous media. *Advances in Water Resources*. Vol. 56, pp. 61–76. DOI: 10.1016/j.advwatres.2013.03.001.

Sequential DeepONets for Predicting Multi-physics Solutions: A Study of Optimal Learning with Multi-inputs

Seid Koric [1,a], Qibang Liu [2], Diab Abueidda[3]

[1] University of Illinois at Urbana-Champaign, E-mail: koric@illinois.edu

[2] University of Illinois at Urbana-Champaign, E-mail: qibang@illinois.edu

[3] University of Illinois at Urbana-Champaign, E-mail: abueidd2@illinois.edu

Deep Operator Networks (DeepONet) [1] approximate linear and nonlinear solution operators by taking parametric functions (infinite-dimensional objects) as inputs and mapping them to solution functions on the computational grid, in contrast to classical neural networks that need retraining or transfer learning for every new set of parametric inputs. Among them, the Sequential DeepONet (S-DeepONet) [2] was recently proposed to use sequential learning models in the branch of DeepONet to simultaneously predict final multi-physics solutions given time-dependent inputs such as transient boundary conditions, loads, or source terms.

This novel study compares S-DeepONet with the single-branch strategy for encoding and coupling multi-inputs [2] to S-DeepONet with the MIONet approach [3], which uses a separate branch for each input. In the first use case, using data from coupled and uncoupled multiphysics finite elements simulations of a solidifying steel domain traveling down the continuous caster in the lagrangian frame of reference, S-DeepONet architectures are trained to predict the final temperature and highly nonlinear stress solution field distributions. This real-world industrial process is responsible for 95% of steel production in the world and is driven by thermal and mechanical temporal boundary conditions on the chilled surface. A comparable investigation in the second example uses

coupled data from the coupled PDE system of electric potential with transient charge distribution and heat conduction with a transient heat source. These PDEs have important applications in thermal management in electronics and semiconductor devices, batteries and energy storage systems, and tissue ablation in biomedical applications, among many others.

Despite different physical phenomena in the examples, it was shown that the solver coupling in classical modeling methodologies in multiphysics can be translated to the newly introduced operator neural network learning, which yields more precise predictions through a single branch that processes and encodes inputs in a coupled manner, utilizing shared trainable parameters. However, the two-branch MIONet model, which processes and encodes inputs in distinct branches before joining them using a tensor product, demonstrated superior performance with uncoupled multiphysics data. When adequately trained, these neural network models may simultaneously predict (inference) multiple multiphysics solution fields up to four orders of magnitude faster than traditional multiphysics computational techniques. This facilitates future design, optimization, inverse and sensitivity analysis, uncertainty quantification, online controls, digital twins, and similar iterative or challenging workflows in engineering, science, and industry that require instant full-field solution evaluations from

---

[a] Presenting Author

computationally intensive and expensive multiphysics analysis for variable boundary conditions, loads, source terms, etc.

Keywords: Multiphysics, Neural Networks, S-DeepONet, Coupling, Multi-Inputs

References:

[1] L. Lu, P. Jin, G. Pang, et al. Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. 2021. Nat Mach Intell 3, 218–229

[2] J. He, S. Kushwaha, J. Park, S. Koric, D. Abueidda, I. Jasiuk. 2024. Sequential deep operator networks (s-deeponet) for predicting full-field solutions under time-dependent loads.

Engineering Applications of Artificial Intelligence, 127:107258

[3] P. Jin, S. Meng, L. Lu. 2022. MIONet: Learning multiple-input operators via tensor product. SIAM Journal on Scientific Computing, 44(6), pp.3490–3514

A 3D Coupled Thermo-Mechanical and Neutron Diffusion Model for Irradiated Concrete

Beatrice Pomaro [1,a], Jiangkun Zhang [1], Gianluca Mazzucco [1], Valentina Salomoni [1]

[1] Department of Civil, Environmental and Architectural Engineering (DICEA) University of Padova (UNIPD)

Via F. Marzolo 9, 35131 Padova, Italy. E-mail: beatrice.pomaro@unipd.it.

Concrete is a highly effective material for nuclear radiation shielding applications [1]. Evaluating the structural performance and integrity of biological shielding throughout the operational lifespan of nuclear facilities requires a thorough investigation of the interconnected physical mechanisms occurring within the shielding material under irradiation. These mechanisms include fast-to-thermal neutron moderation, temperature increases due to radiation absorption, radiation-induced volumetric expansion (RIVE), and more.

To address these aspects, a fully coupled three-dimensional thermo-mechanical and neutron diffusion (TMN) model is proposed. This numerical model is developed within the framework of the Finite Element Method (FEM) [2], allowing the study of cementitious materials both at the homogeneous scale and the mesoscale. The mesoscale approach is particularly advantageous for capturing radiation-induced antagonistic effects between aggregates and mortar.

The TMN model incorporates a two-group neutron diffusion theory coupled with heat conduction, accounting for thermal neutron capture. In the mechanical domain, it integrates visco-elasto-plasticity and damage mechanisms [3], providing an effective framework to model the key interactions between radiation-induced effects and material nonlinearities.

Keywords: Concrete; Nuclear radiation; Coupling; Multi-physics; Radiation damage.

References:

[1] M.F. Kaplan. 1989. Concrete radiation shielding: Nuclear physics, concrete properties, design, and construction, John Wiley & Sons Ltd, New York.

[2] J. Zhang, B. Pomaro, G. Mazzucco, B. F. Dongmo, C. Majorana, and V. Salomoni. 2024. A 3D coupled thermo-mechanical and neutron diffusion numerical model for irradiated concrete. Int. J. Mech. Sci., Vol. 264, pp. 108806.

[3] G. Mazzucco, B. Pomaro, B.F. Dongmo, V. Salomoni, C. Majorana. 2022. Combined 3D visco-elasto-plasticity and damage to model fatigue in concrete. 15th World Congress on Computational Mechanics (WCCM-XV) 8th Asian Pacific Congress on Computational Mechanics (APCOM-VIII) 31 July – 5 August 2022, Yokohama, Japan.

[a] Presenting Author

Improving alpine skiing performance through video analysis of the ideal and real

Denisa-Iulia Brus [1,a], Dorin-Ioan Cătană [2]

[1] Transilvania University, E-mail: denisa.brus@unitbv.ro

[2] Transilvania University, E-mail: catana.dorin@unitbv.ro

In the current context of the digital era, the field of sports training is about to undergo a profound transformation, with significant implications for athletes. This imminent change has led to the development of an innovative application designed to enhance athletes' performance through video monitoring of training sessions. The application of advanced technologies in training supervision and analysis provides the opportunity to obtain precise and immediate feedback, thereby facilitating the adjustment and optimization of training techniques to maximize athletes' performance. This initiative represents an important step in integrating technology into the sports training process, contributing to the evolution of training methodologies and achieving superior results.

The OptiPath application represents an absolute novelty in alpine skiing. Its innovation lies in the fact that, until now, there has been no application designed to compare the ideal path with the actual one. OptiPath includes both established elements from the field as well as new aspects, or those assimilated from related fields, to fully achieve the initial objectives set

OptiPath is an innovative desktop application designed to enhance alpine skiing performance by analyzing and comparing the skier's path to an ideal trajectory. Utilizing Python for development, the application integrates cutting-edge image processing, machine learning, and artificial intelligence techniques to detect gates, track skier movement, and calculate the optimal path. A mathematical model based on the physics

of skiing ensures precise trajectory computation, enabling athletes and coaches to identify areas for improvement.

The application is built on a "Smart Client" architecture, ensuring smooth user interaction and requiring minimal system resources, making it both accessible and efficient. Currently in its early stages of development, OptiPath demonstrates significant potential for enhancement. By incorporating IMU (Inertial Measurement Unit) sensors, the application could achieve higher accuracy, offering skiers detailed data to fine-tune their techniques and improve performance. This potential positions OptiPath as a valuable tool for both professional and recreational skiers striving to maximize their results on the slopes.

Keywords: alpine skiing, ideal skiing path, alpine skiing application

[a] Presenting Author

References:

[1] U.D. Jentschura, F. Fahrbach. 2004. Physics of skiing: The ideal–CARVing equation and its applications. Canadian Journal of Physics. Vol. 84, pp. 249-261.

[2] R. Neptune. 2000. Computer Modeling and Simulation of Human Movement: Applications in Sport and Rehabilitation. Physical Medicine and Rehabilitation Clinics of North America. Vol. 11, pp. 417-434.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

A Domain Decomposition Multi-Scale Method for Simulation in Direct Energy Deposition Additive Manufacturing

Patricia Barral[12], Miguel Picos[12,*], Peregrina Quintela[12], Jer´onimo Rodrguez[12]

[1] Centro de Investigaci´on y Tecnolog´ıa Matem´atica de Galicia (CITMAGA); Campus Vida, Technological Research Institute; Ru´a de Constantino Candeira, s/n, 15782 Santiago de Compostela, Spain; E-mail:

citmaga@citmaga.gal; https://citmaga.gal/en/home

[2] Departamento de Matem´atica Aplicada, Universidade de Santiago de Compostela (USC); Campus Vida, Facultad de Matem´aticas; Ru´a Lope G´omez de Marzoa, s/n, 15782 Santiago de Compostela, Spain; E-mail:

departamento.matematicaaplicada@usc.gal;

https://www.usc.gal/en/department/applied-mathematics

Abstract: Additive Manufacturing (AM) is an advanced production technique that is growing in the manufacturing industry. AM is based in material addition instead of the classical subtraction techniques. This brings new capabilities to the manufacturing processes, such as, reduce in material and energy wastage, freedom in design or personalized designs for small batches. One of the many technologies that conform AM is the Direct Energy Deposition (DED), based on producing metallic pieces by continuously adding material as a heat source melts it, forming the desired piece.

DED AM uses high power heat sources, becoming one of the fastest existing metallic AM technologies. In addition, as the material and energy are supplied simultaneously by a robotic header, there are no limitation in piece sizes due to closed compartments, as other AM technologies have. This also allows DED AM to be suitable for repairing purposes, as a damage piece can be restored by applying additional material to the damage area. Repair costs are significantly lower than the cost of new manufacturing, opening new opportunities for this technology to expand its role in the manufacturing industry.

DED AM also faces some challenges due to the high power heat sources involved. Right below the heat source, the metallic feedstock, powder or wire, is melted in a small period of time. That forms a melted pool where liquid metal can freely move. As the manufacturing process progresses, the heat source moves, moving the melt pool with it. The movement of the melt pool comes from new material that is being melted and added to the melt pool and material from the melt pool that cools down to solid state, forming the desired geometry of the piece. This makes the process intrinsically multi-physic as fluid dynamics, heat evolution, phase change and mechanical evolution, due to heat gradients, are involved in the manufacturing process.

Heating and cooling processes happen in small parts of the piece, under the heat source and in small periods of time. This creates high thermal gradients in the piece that leads to mechanical deformations and residual stresses that accumulate over the full piece during the whole manufacturing process. There are two main research fields in DED AM: micro scale and macro scale levels. The micro scale research studies what happen in the surroundings of the melt pool and the macro scale one studies the global behaviour of the piece. The first one focus on heat evolution, fluid dynamics and phase changes while

the second one focus on heat evolution and mechanical deformations. We are focused in the second orientation of research.

One of the main challenges for DED AM at the moment is deformation on big pieces, as there is no useful tool to predict it. Trial and error strategies are still state of the art in this field, highly increasing costs. Simulation is key to optimize deposition strategies in order to reduce or counter deformations and overheating. Although there are some techniques to make simulations on these manufacturing processes, such as the quiet element method or the inactive element method [1], they are not well suited for large pieces. The temporal and spatial multi-scale of the problem increase the computational cost so much that simulations are no longer worth. Our work presents a numerical approach focused on reducing computational costs.

DED AM simulation main challenges are the multi-scale of the problem and the continuous addition of material. To face the first one, a domain decomposition technique, based on the Arlequin method, is proposed. It uses two meshes with different degrees of refinement, for critical and non-critical regions, so that the total degrees of freedom are reduced. This method does not require congruent meshes, bringing the possibility for the fine mesh to move with the heat source in a continuous smooth way.

Taking advantage of a mesh that moves with the heat source, and where new material is added, we adopt a reference frame transformation over the finer mesh to implicitly account for the continuous growth of the domain. This can only account for a local increase of the domain, so we also use the Finite Addition of Matter Elements (FAME) method, introduced in [2], based on interchanging information between meshes so that new elements of the global coarser mesh inherit the temperatures from the finer moving

mesh. Combining these strategies we are able to deal with the continuous growth of the domain, without relying on user defined

element initialization.

The validation of the proposed method is carried out through a comprehensive set of analytical tests, designed to evaluate behaviors observed in real applications, and supported by experimental data.

Keywords: Additive Manufacturing, Domain Decomposition, Multi-scale Methods, Arlequin Methods, Finite Element Method

---

* Presenting author

References

[1] Michaleris, P. (2014). Modeling metal deposition in heat transfer analyses of additive manufacturing processes. *Finite Elements in Analysis and Design*, 86, 51-60.

[2] Ruyssen, R. and Ben Dhia, H. (2022). A finite addition of matter elements method for modeling and solution of an SLM thermal problem by a multiscale method. *International Journal for Numerical Methods in Engineering*, 123(8), 1760-1790.

Self-Attention-Enhanced LSTM Model for Metro Station Passenger Flow Prediction: Accuracy and Performance Analysis

Yuyang Shao[1]; S. Thomas Ng[2,a]; Ruiyan Zheng[3]; Yifan Yang[4];
C. Y. Kwok[5]; Reynold Cheng[6]
[1] City University of Hong Kong, E-mail: Y.Y.Shao@cityu.edu.hk
[2] City University of Hong Kong, E-mail: thomasng@cityu.edu.hk
[3] Dalian University of Technology, E-mail: zhengruiyan@mail.dlut.edu.cn
[4] Nanjing University of Aeronautics and Astronautics, E-mail: yifan.yang@nuaa.edu.cn
[5] University of Hong Kong, E-mail: fkwok8@hku.hk
[6] University of Hong Kong, E-mail: ckcheng@cs.hku.hk

Accurate forecasting of short-term metro station passenger flow is essential for effective transportation planning and operational management. Long Short-Term Memory (LSTM) networks are widely utilized for such tasks due to their strong capability in modeling temporal patterns within sequential data. However, their effectiveness can be limited by challenges in capturing long-range dependencies, which may adversely affect prediction accuracy. To address this limitation, this study introduces a self-attention-enhanced LSTM model that dynamically prioritizes the most relevant input features to improve predictive performance. The proposed model integrates multiple sources of data, including historical passenger flow data, station characteristics, and holiday effects, to comprehensively capture critical data features while analyzing predictive performance across various scenarios. Experiments conducted on data from the Hong Kong Mass Transit Railway (MTR) demonstrate that the self-attention-enhanced model achieves lower Mean Absolute Error (MAE) and Root Mean Squared Error (RMSE) compared to the standard LSTM model. These results underscore the potential of the enhanced model to deliver more accurate

passenger flow predictions, which facilitates better transit system management and decision-making.

Keywords: Passenger flow prediction; deep learning; long short-term memory; self-attention mechanism; multi-source data

[a] Presenting Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Accelerating Multi-Scale Simulations using Uncertainty-Driven Phase-Field Mixtures of Constitutive Models

J. Storm[1,*], W. Sun[2], I. B. C. M. Rocha[1], F. P. van der Meer[1]

[1]Delft University of Technology

[2]Columbia University

*Email: j.storm@tudelft.nl

Abstract: Accelerating multi-scale models using data-driven techniques is a rapidly evolving research field. While surrogate models offer promising speedups for multiscale simulations, creating comprehensive training datasets that capture the constitutive behavior for all loading conditions remains computationally intensive. We propose an adaptive mixture methodology that combines a fast surrogate and the original model it was trained to replace. This approach eliminates the requirement for surrogate accuracy across all possible loading scenarios, substantially reducing the data generation burden. We implement this by introducing phases in the computational domain, corresponding to the original constitutive model and the surrogate. The choice for a probabilistic surrogate makes it possible to let these phases evolve through a phase-field driven by the surrogate uncertainty. When the uncertainty increases, the phase-field gradually switches the constitutive model from the surrogate to the original model. We discuss the requirements of this approach to achieve accurate and stable results and compare the phase-field to a purely local approach that does not enforce spatial smoothness. Through numerical examples, we demonstrate how this mixture of models can accelerate multi-scale simulations.

Keywords: Surrogate modeling, Adaptive modeling, Phase-field, Gaussian Process

---

* Presenting author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Numerical Assessment of Thermal Insulation System of a 6 CBM Liquid Hydrogen Fuel Tank for Maritime Applications

D.H. Hong [1,a], G.W. Kim [2], H.S. Kim [3], S.Y. Kim [4]

[1] Korea Research Institute of Ships and Ocean Engineering, E-mail: davis.hong@kriso.re.kr

[2] Korea Research Institute of Ships and Ocean Engineering, E-mail: gwkim@kriso.re.kr

[3] Korea Research Institute of Ships and Ocean Engineering, E-mail: hskim85@kriso.re.kr

[4] Hylium Industries Inc., E-mail: seokim@hylium-industries.com

This study conducted a numerical analysis to evaluate the thermal insulation performance of a liquid hydrogen (LH2) fuel tank designed for maritime applications. Hydrogen, widely regarded as a sustainable fuel due to its zero carbon emissions, presents significant challenges in storage and transportation owing to its low volumetric energy density. To address these challenges, various hydrogen storage technologies have been developed, with LH2 emerging as a particularly promising solution. However, its cryogenic liquefaction temperature necessitates advanced insulation technologies, particularly for marine applications that must withstand dynamic and harsh environmental conditions.

The insulation system developed for a 6-cubic-meter LH2 fuel tank was introduced, which has received Approval in Principle (AIP) certification by KR (Korean Register). The system utilizes multilayer insulation (MLI) installed between vacuum layer between inner and outer vessel, as the primary insulating material. To further enhance thermal performance, a vapor-cooled shield (VCS) and a heat dissipation structure leveraging vaporized hydrogen at cryogenic temperatures were integrated. The thermal insulation system was analyzed using computational fluid dynamics (CFD) methods, and the results demonstrated that the VCS-integrated insulation system reduced total heat penetration by up to 20%.

Acknowledgement: This research was supported by the grant from National R&D Project "Research Hub Establishment and International Joint Research on Advanced Maritime Mobility (AMM) between Korea and Europe" funded by Ministry of Oceans and Fisheries (RS-2024-0041020).

Keywords: Liquid Hydrogen, Fuel tank, Vapor cooled shield, boil-off rate, Computational Fluid Dynamics

---

[a] Presenting Author

References:

[1] J. Zheng, L. Chen, J. Wang, Y. Zhou, J. Wang. 2019. Thermodynamic modelling and optimization of self-evaporation vapor cooled shield for liquid hydrogen storage tank. Energy Conversion and Management. Vol. 184, pp. 74-82.

신정용/친환경연료추진연구센터/2025-01-24 12:02

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Using Computer Vision to predict microscale turbulent drag force in porous media

Vishal Srikanth [1] , Andrey V. Kuznetsov [1,a]

[1]Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC 27695, USA

Convolution Neural Networks (CNN) are well-suited to model the nonlinear relationship between the microscale geometry of porous media and the corresponding flow distribution, thereby accurately and efficiently coupling the flow behavior at the micro- and macro- scale levels. In this work, we have identified the challenges involved in implementing CNNs for macroscale model closure in the turbulent flow regime, particularly in the prediction of the drag force components arising from the microscale level. We report that significant error is incurred in the crucial data preparation step when the Reynolds averaged pressure and velocity distributions are interpolated from unstructured stretched grids used for Large Eddy Simulation (LES) to the structured uniform grids used by the CNN model. We show that the range of the microscale velocity values is 10 times larger than the range of the pressure values. This invalidates the use of the mean squared error loss function to train the CNN model for multivariate prediction. We have developed a CNN model framework that addresses these challenges by proposing a conservative interpolation method and a normalized mean squared error loss function.

To develop the CNN model framework, we chose to simulate the dataset for a model problem

of turbulent flow in periodic porous media composed of cylindrical solid obstacles with a square cross-section. We varied the porosity of the porous medium in the range 0.3 to 0.88 to generate 61 samples. The samples include a wide range of flow behaviors encompassing two unique flow regimes: the low and intermediate porosity flow regimes, which are characterized by recirculating and shedding vortex structures respectively. The validation of the CNN model trained with the present dataset revealed the following challenges hindering the development of macroscale closure models with this approach.

The first challenge is introduced by the need to predict multiple variables (pressure and velocity) in order to calculate the pressure and viscous drag force components. For turbulent flow in porous media, the values of microscale pressure and velocity inside the pores span different ranges, such that the range of streamwise velocity values is an order of magnitude larger than the range of the pressure values. Therefore, the CNN model trained using the popular Mean Square Error (MSE) loss function results in the model learning to accurately predict only the streamwise velocity distribution since the magnitude of streamwise velocity is typically larger than that of the pressure. To overcome this, we used a normalized loss function to train the CNN model such that each component of the CNN model output is normalized with respect to its mean value. We demonstrated the use of the normalized MSE loss function in our CNN model decreased the model error in the simultaneous prediction of pressure and streamwise velocity by a factor of 4.

The second challenge is introduced by the need to interpolate the turbulence dataset from an

unstructured grid used for LES to a structured grid of a specified size that is compatible with the CNN model. The interpolation error is compounded when the first and second derivatives

of pressure and velocity are calculated to compute the drag force. Significant interpolation error is introduced by linear interpolation methods, especially in the near-wall regions where the LES grid is stretched to resolve the turbulent boundary layer. We evaluated two possible solutions to overcome this challenge. In the first solution, the error caused by the linear interpolation method is minimized by using a fine structured grid for interpolation and then upscaling the interpolated flow distribution to a coarse grid that is compatible with the CNN model. This approach decreased the error in the prediction of pressure drag by a factor of 10 (from 101% to 10.4%) when compared to the coarse grid linear interpolation. However, the estimation of the viscous drag continued to have substantial interpolation error. We addressed this in the second solution by using a conservative interpolation scheme that satisfies the macroscale governing equation of momentum on both the unstructured LES grid and the structured CNN grid. By using the conservative interpolation approach, we decreased the interpolation error in the CNN model to virtually zero for both the pressure and viscous drag calculations.

In summary, we have developed a CNN model framework that processes turbulent flow data simulated by LES and then trained the model to predict the density of the momentum sources of the pressure and viscous drag forces. By using the proposed conservative interpolation method and the normalized MSE loss function, the resulting CNN model predicts the pressure and viscous drag forces with less than 10% mean absolute error over the range of porosities from 0.3 to 0.88. The CNN model offers a speedup in the calculation of the drag force components of $O(10^6)$ when compared to LES, where the CNN model takes less than 0.4 seconds on a

desktop computer and the LES took 2 months of computation time on a linux cluster. Further development of the CNN model for turbulent flow in porous media with a more robust dataset holds tremendous potential for the design and modeling of optimized porous materials.

Keywords: neural networks, numerical methods, tube banks

---

[a] Presenting Author

Molecular Dynamics Simulation of Deposition and Nanoindentation in SiNx/BNy Amorphous Periodic Nanolayered Coatings: Insights into Growth and Strengthening Mechanisms

Pengyuan Wu[1,a], Oleksiy V. Penkov [1]

[1] Zhejiang University, E-mail: pengyuan.22@intl.zju.edu.cn

[1] Zhejiang University, E-mail: oleksiypenkov@intl.zju.edu.cn

Deposition of periodical nano-layered coatings (PNCs) using magnetron sputtering is a practical approach to enhance the durability of optical components. The mechanical properties of PNCs are influenced by structural factors such as modulation period and thickness ratio, with the strengthening mechanism closely tied to the inhibition of strain propagation at heterogeneous interfaces. In our previous studies, we developed SiNx/BNy PNCs consisting of alternated SiNx and BNy layers. These coatings exhibited a hardness of up to 32.4 GPa, significantly higher than that of single-component SiNx or BNy coatings, while also demonstrating excellent flexibility.

In this study, we employed molecular dynamics (MD) simulations to model the deposition process of the coatings, achieving SiNx/BNy PNCs models with different layer thicknesses that align well with experimental observations. We also investigated the effect of the incident kinetic energy of atoms on component density and interlayer mixing, with simulation results matching experimental data. Based on the established SiNx/BNy PNCs models, MD simulations were used to study the nanoindentation process. The simulations revealed that, for a fixed SiNx thickness, the coating hardness is strongly dependent on the thickness of the BNy layer. This phenomenon can be attributed to the fact that thin BNy layers fail to

form distinct interfaces with SiNx, while thicker BNy layers enhance interfacial obstruction to strain propagation. Conversely, when the BNy layer becomes excessively thick, the mechanically weaker BNy layer undergoes significant strain due to compression from the overlying SiNx layer, leading to enhanced strain propagation and stress concentration, which ultimately reduces the coating's hardness. Accurate nanoindentation tests validated the simulation results.

These findings provide valuable insights into the structural design of PNCs, paving the way for further optimization of their mechanical performance.

Keywords:

Periodical nanolayered coating, magnetron sputtering, molecular dynamics simulation, amorphous coatings.

[a] Presenting Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Design of the Cryogenic Liquefied Hydrogen Corrugated Tank using Topology Optimization and Thermal Stress Analysis

Song-Hyun Cha [1,a] Gun Woo Kim [1], Ha-yeong Kim[1], Hyun-seok Kim [1]

[1] Korea Research Institute of Ships and Ocean Engineering, E-mail: shcha0808@kriso.re.kr

Since fossil fuels cause global warming, alternative energy development is needed. Hydrogen energy is one of the most representative alternative energies. In order to use the hydrogen energy, advanced heat insulation technology is required for long-term at ultra-low temperature of 20K. In order to delay the vaporization of liquefied hydrogen in the tank, the heat transfer between inner tank and outer tank through supporters should be minimized. In addition, the load of the inner tank and the liquefied hydrogen should be withstood by them. Inside the tank, large temperature difference cause significant thermal deformation and thermal stress. To improve this situation, the corrugated structure was introduced, which relieves thermal stress concentration. In this paper, the shape of the supporters, and the dimension of the tank were determined by topology optimization and thermal stress analysis to complete the design.

Topology optimization is used for the mechanical property. Topology optimization method is proposed, minimizing structural compliance. The problem is posed as a two-phase layout problem where the phases include an insulating material, G10 and the structural material, stainless steel 316L. Since the

optimization proceeds in the direction of decreasing mass, thermal conductivity of the optimal design also decreases. Thus, it minimizes heat inflow from outer tank to inner tank while ensuring structural performance.

The temperature distribution on the tank was obtained by CFD using STAR-CCM+, and the thermal stress analysis was performed using ANSYS. Based on the results, the curvature of the corrugated structure, the thickness of the plate were partially modified, and this process was repeated to confirm the final storage tank design withstood the load.

Keywords: Liquefied hydrogen, Topology optimization, Liquefied hydrogen storage tank, Thermal stress analysis

Acknowledgement: This research was supported by the grant from National R&D Project "Research Hub Establishment and International Joint Research on Advanced Maritime Mobility(AMM) between Korea and Europe" funded by Ministry of Oceans and Fisheries(RS- 2024-0041020).

[a] Presenting Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Towards second-order FE^2 multiscale solutions for quasi-stationary thermal problems with a heterogeneous heat source

Isabelle Rami`ere[1,*], Louis Belgrand[1,2] and Fréderic Lebon[2]

[1] CEA, DES, IRESNE, DEC, SESC ; Cadarache, F-13108 Saint-Paul-Lez Durance, E-mail: isabelle.ramiere@cea.fr

[2] Aix-Marseille Universit´e, CNRS, Centrale Marseille, LMA ; F-13453 Marseille cedex 13, E-mail: lebon@lma.cnrs-mrs.fr

Abstract:

In this work derived from [1], we focus on the multiscale resolution of a (quasi-)stationary thermal problem with a source term in a heterogeneous material. This scenario differs from the mechanical computational homogenization framework in that it seeks a precise primal solution (temperature) on the Representative Volume Element (RVE), and also considers a source term, which may be heterogeneous at the microscale.

Various Finite Element square (FE^2) approaches are reviewed, primarily differing in their treatment of the source term within the microstructure. These approaches are analyzed and compared theoretically, particularly by drawing parallels with methods based on double-scale asymptotic expansions.

For this problem, the classical FE^2 method [3] adheres to the Hill-Mandel principle and does not impose a source term on the microstructure. Consequently, the method is of first order and does not account for local temperature variations due to the source within the microstructure. In cases with low or no insulated inclusions, these approaches have proven sufficiently accurate. However, when insulating inclusions are present, it becomes crucial to consider the local influence of the source term in order to obtain accurate solutions at the microscale [2]. Recently, the generalized Hill-Mandel principle [4, 5] has been introduced,

enabling the inclusion of the source term within the microstructure in a FE^2 framework. We show that this strategy results in methods of higher than first-order accuracy.

The accuracy of the numerical results obtained by these different approaches is evaluated through direct simulation of the structure, discretizing the heterogeneities. This study concludes that it is essential to consider the complete heat source within the microstructure [5], rather than only its fluctuations [4], to obtain reliable estimates of temperature variations at this scale.

Finally, a quasi-stationary FE^2 calculation with temporal loading and nonlinear behavior has been success- fully performed. This calculation represents a nuclear fuel irradiation scenario, in which coupling with other physical processes is carried out at the macroscopic scale. The simulation confirms the importance of us- ing the generalized Hill-Mandel principle to avoid underestimating the temperature in the microstructural inclusions.

Keywords: Heterogeneous material, Computational Homogenization, Asymptotic expansion, Generalized Hill-Mandel principle, Finite element square

* Presenting author

References

[1] L. Belgrand. *On the accuracy of microscale solutions in modeling the multiscale thermo-mechanical behavior of heterogeneous materials*. PhD thesis, Aix-Marseille University, 2023.

[2] J. F. Bourgat. Numerical experiments of the homogenization method. In R. Glowinski, J. L. Lions, and I. Laboria, editors, *Computing Methods in Applied Sciences and Engineering, 1977, I*, pages 330–356, Berlin, Heidelberg, 1979. Springer Berlin Heidelberg.

[3] G. Chatzigeorgiou, N. Charalambakis, Y. Chemisky, and F. Meraghni. Periodic ho- mogenization for fully coupled thermomechanical modeling of dissipative generalized standard materials. *International Journal of Plasticity*, 81:18–39, 2016.

[4] E. A. de Souza Neto, P. J. Blanco, P. J. Sa´nchez, and R. A. Feij´oo. An RVE-based multiscale theory of solids with micro-scale inertia and body force effects. *Mechanics of Materials*, 80:136–144, 2015.

[5] G. R. Ramos, T. dos Santos, and R. Rossi. An extension of the Hill–Mandel principle for transient heat conduction in heterogeneous media with heat generation incorporating finite RVE thermal inertia effects. *International Journal for Numerical Methods in Engineering*, 111(6):553–580, 2017.

Multi-physics, multi-scale modelling of droplet behaviour in an electric field

Alex Martynenko

Department of Engineering, Dalhousie University, Truro, NS B2N 5E3, Canada

alex.martynenko@dal.ca

Recent advancements in electrotechnologies, such as electrospinning, electrospraying, electrowetting, electrocoalescence, and electrohydrodynamic cooling, have sparked significant interest in understanding the behavior of water droplets in electric fields. The study of droplet motion, deformation, and disintegration under electric fields is inherently challenging due to the coupling of heat, mass, momentum, and charge transfer. Consequently, numerical simulations using multi-physics and multi-scale approaches are crucial.

The advent of advanced computational methods provides a unique opportunity to simulate droplet dynamics under electric fields. Prior studies, such as those by Hosseini et al. [1] and Liu et al. [2], have demonstrated the effects of electric fields on droplet motion and deformation, considering surface tension, gravity, and electrostatic forces. However, many aspects of these phenomena remain insufficiently understood.

This study focuses on the liquid-air interface dynamics of a single water droplet subjected to a vertical electric field. A two-dimensional numerical model was developed using COMSOL 5.6 (COMSOL Inc., MA, USA), employing the Finite Element Method (FEM). The Maxwell stress tensor components were incorporated to quantify the effects of the electric field, and a phase-field analytical method was applied to model the two- phase flow with moving boundaries. This approach effectively captures the density transitions at the liquid-air interface.

Our results highlight the dominant influence of electrostatic (Coulomb) force on droplet motion, deformation and disintegration. Simulations of electroconductive and purely dielectric droplets revealed that the droplet response time to the electric field decreases exponentially with increasing field strength and droplet size. For instance, the 1 mm droplet response time was 107 ms. Additionally, the electric field induced horizontal motion in droplets—a critical factor in applications like surface cleaning. This displacement increased with droplet size but exhibited an optimal threshold relative to the applied voltage.

In summary, the motion of droplets in a uniform electric field depends on the fluid viscosity, gravity, and electrostatic forces. In non-uniform electric fields, an additional dielectrophoretic force directs droplets toward regions of higher electric field strength. In the ionization region, electric fields ionize water molecules, leading to faster droplet disintegration due to the electrostatic repulsion of unipolar charges. Our study provided new insights into the mechanisms governing droplet behaviour in uniform and non- uniform electric fields.

Keywords: electrotechnology, simulation, water droplet, liquid-air interface

1. Hosseini, M., Arasteh, H., Afrouzi, H. H., & Toghraie, D. (2020). Numerical simulation of a falling droplet surrounded by air under electric field using VOF method: A CFD study. *Chinese Journal of Chemical Engineering*, 28 (12), 2977-2984.Liu, R., Wang, Y. B., Xie, F. F., Yang, S. W., Liu, H. W., Yang, Y. R., Lee, D. J. (2021).

Bouncing dynamics of a nanodroplet impacting a superhydrophobic surface under perpendicular electric fields. *Colloids and Surfaces: Physicochemical and Engineering Aspects*, 630, 127617.

Automated Characterization of Debonding based on Ultrasonic Guided Waves and A Simulation-Trained Deep Neural Network

Jianmin Qu [1,a] Junzhen Wang[2]

[1] Stevens Institute of Technology, E-mail: Jianmin.Qu@Stevens.edu

[2] Iowa State University, E-mail: junzhenw@iastate.edu

This article proposes an automated nondestructive evaluation (NDE) technique for debonding characterization using ultrasonic guided waves and a simulation-trained deep neural network. This technique is based on guided waves generated and received in a transmitter- receiver configuration. First, finite element simulations are conducted to obtain time-series pulse-echo and pitch-catch debonding responses. These signals serve as training data for a hybrid neural network that combines a convolutional neural network (CNN) with a bi-directional long short-term memory (BiLSTM) layer. Once trained, this deep-learning model is able to automatically characterize the location and size of debonding damage by inputting either simulated or experimentally measured guided wave signals. The developed deep-learning model is validated by conducting guided wave active sensing experiments on a pristine plate and four debonding specimens with various debonding locations and sizes. The experimental results demonstrate that the developed neural network, once

trained, is capable of accurately characterizing debonding sizes. These findings indicate that the proposed technique has tremendous potential for characterizing interfacial debonding in practical NDE and structural health monitoring (SHM) applications.

Keywords: Guided wave; debonding; deep neural network; nondestructive evaluation; structural health monitoring

[a] Presenting Author

Advancements in GS4-*i*-ROM: a unified time integration for coupled first-second order time-dependent problems

Tao Xue*[1], Yazhou Wang[2], Xiaobing Zhang[3], and Kumar Tamma[4]

[1] Nanjing University of Science and Technology, Nanjing, Jiangsu, 210094, PR China, E-mail: tao.xue@njust.edu.cn

[2] Technical University of Munich, Garching, Munich 85748, Germany, E-mail: yazhou.wang@tum.de

[3] Nanjing University of Science and Technology, Nanjing, Jiangsu, 210094, PR China, E-mail: 906868624@qq.com

[4] University of Minnesota Twin Cities, MN 55455, United States of America E-mail: ktamma@umn.edu

Over the years, there has been significant progress in the development of time integration algorithms for solving time-dependent problems in computational mechanics. These algorithms play a crucial role in solving first-order transient systems (e.g., fluid dynamics, heat transfer) or second-order transient systems (e.g., structural dynamics, wave propagation). Notable examples of these algorithms include LMS, composite method, and time finite element method. In previous research, Tamma's group introduced the Generalized Single-Step Single-Solve Isochronous time integration (GS4 *i*-integration) approach. This innovative method allows for the direct solution of both first-order and second-order transient systems, as well as their coupled systems, without relying on separate frameworks. The GS4 *i*-integration is based on a three-root system that utilizes the *u*-*v*-*a* set of variables to adapt the two-root system (*u*-*v* system), resulting in the inclusion of a dummy variable in the scheme.

In this study, we present an alternative perspective on the GS4 *i*-integration that starts from the *u*-*v* system and naturally extends to cover the *u*-*v*-*a* systems. By adopting this approach, all physics fields in both first-order and second-order systems are naturally incorporated without the need for dummy variables. We demonstrate that by tuning only two algorithmic parameters, desirable numerical features such as energy conservation, controllable numerical dissipation, second-order accuracy, and zero-order overshoot can be achieved. Furthermore, we integrate the proposed isochronous schemes with the proper orthogonal decomposition (POD) technique to create a unified model order reduction framework, called GS4-*i*-ROM. This framework enables the solution of coupled problems under a single analysis, incorporating the widest set of optimal and compatible algorithms. To illustrate the effectiveness of our approach, we apply it to classical one-way and two-way coupled thermoelastic problems. Through these examples, we demonstrate the adaptive procedure and numerical performance of the GS4-*i*-ROM approach, highlighting its improved efficiency in solving coupled problems. Ultimately, our goal is to implement the GS4-*i*-ROM approach in studying structure/thermal/fluid interactions within the field of computational mechanics, thereby enhancing the accuracy, efficiency, and robustness of numerical simulations involving coupled physics.

Keywords: Reduced order modelling, GS4 *i*-integration, coupled systems

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Optimal solutions and r-adaption employing an algebraic Variational Multiscale approach

Suyash Shrestha[1,2,*], Marc Gerritsma[2], Gonzalo Rubio[1], Steven Hulshoff[2], Esteban Ferrer[1]

[1]ETSIAE-UPM-School of Aeronautics, Universidad Polit´ecnica de Madrid, E-mail: s.shrestha@upm.es; s.shrestha-1@tudelft.nl

[2]Delft University of Technology, Faculty of Aerospace Engineering

Abstract:

This work presents an algebraic Variational Multiscale (VMS) framework for tackling non-linear problems such as Burgers' and incompressible Navier-Stokes equations. Building upon the methodologies established in [1] and [2], the present work serves to provide a generalisation towards non-linear problems and a demon- stration of the efficacy of the proposed framework for mesh adaption. The VMS formulation is derived based on the projector defined using the energy norm associated with the symmetric part of the differential oper- ator. We refer to this projector as the optimal projector and present a discretisation approach that yields a numerical solution closely approximating the optimal projection of the infinite-dimensional continuous/DNS solution. We inherit the approach for linear problems presented [2] which involves solving the VMS problem on two separate meshes: a coarse mesh on which the resolved scales are computed and a fine mesh where the unresolved scales are approximated using the Fine-Scale

Greens' function [1]. The proposed extension is demonstrated through its application to Burgers' equation and the incompressible Navier-Stokes equations in two dimensions. In addition to the theoretical developments, this study showcases one possible application of the VMS framework, namely r-adaptation. We employ an adaption strategy whereby the mesh nodes are dynamically redistributed over the computational domain to capture localised solution features. The results demonstrate how the approach can automatically adapt the computational mesh in response to computed unresolved scales. The demonstration highlights its potential for practical use in adaptive computational techniques and further highlights the effectiveness of the VMS framework in delivering solutions that closely approximate the optimal projection of the infinite-dimensional continuous/DNS solution.

Keywords: Optimal projections; Variational Multiscale; Fine-Scale Greens' function; Spectral Element Method; r-adaption; Burgers' equation; Navier-Stokes equation

---

* Presenting author

References

[1] S. Shrestha, J. Dekker, M. Gerritsma, S. Hulshoff, I. Akkerman, Construction and ap- plication of an algebraic dual basis and the Fine-Scale Greens' Function for computing projections and reconstructing unresolved scales,

Computer Methods in Applied Me- chanics and Engineering 422 (2024) 116833.

[2] S. Shrestha, M. Gerritsma, G. Rubio, S. Hulshoff, E.Ferrer, Optimal solutions employing an algebraic Variational Multiscale approach Part I: Steady Linear Problems, ArXiv (2024) 2409.05231.

Coupled multi-physics simulation of light-material interaction in additive lithography for electronics

Marwan Aarab[1,a], Marc G.D. Geers[1], Joris J.C. Remmers[1]

[1] Eindhoven University of Technology m.aarab@tue.nl

In stereolithography, a resin is cured through UV light exposure. During this process, the resin's optical properties evolve, creating a two-way coupling between light propagation and material curing. One emerging application is 3D additive lithography for electronics (3D-ALE), which integrates microelectronics and chip packaging by combining high-resolution direct lithography with conductive metal paste deposition [1].

Achieving microscale curing accuracy is critical for 3D-ALE. However, printing on various substrates and embedding conductive tracks introduce complex optical phenomena, including photobleaching, scattering, reflection, and absorption. Most models in stereolithography literature do not fully capture these effects. Current light simulation tools lack efficient coupling with multi-physics models and do not capture all of the aforementioned optical phenomena.

To address this, we developed a GPU-accelerated volumetric ray tracing engine for modeling light-material interactions in stereolithography. The tool analyzes rough reflections from embedded metal tracks, substrates, and previous layers. It is tightly coupled with a Finite Element Method (FEM) simulation [2], forming a two-way interaction: the ray tracer provides spatial light absorption data for curing kinetics, while the evolving curing state modifies the resin's optical properties, dynamically altering light propagation. The ray tracer is designed for seamless integration into multi-physics simulations and features tailored intersection acceleration algorithms for computational efficiency [3].

Keywords: Volumetric Ray Tracing, FEM, GPU acceleration, Stereolithography, Micro- electronics

[a] Presenting Author

References:

[1] J. A. H. P. Sol, M. Aarab, W. van Grondelle, D. R. Walsh, S. C. E. Suijdendorp, J. J. C. Remmers, and H. B. Akkerman, "High-resolution additive manufacturing for 3d multifunctional microelectronic devices," in *Proceedings of SPIE Photonics West*, (San Francisco, California, US), 2025.

[2] S. Westbeek, J. J. C. Remmers, J. A. W. van Dommelen, and M. G. D. Geers, "Multi-scale process simulation for additive manufacturing through particle filled vat photopolymerization," *Computational Materials Science*, **vol. 180**, p. 109647, 2020, doi: 10.1016/j.commatsci.2020.109647.

[3] M. Aarab, M. G. D. Geers, and J. J. C. Remmers, "Efficient accelerated volumetric spectral ray tracing engine for coupled multi-physics simulations," *manuscript in preparation*.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Chance constrained optimization of gas transport using kernel density estimation

Hendrik Wilka[1,*], **Jens Lang**[2]

[1]Technical University of Darmstadt, E-mail: wilka@mathematik.tu-darmstadt.de

[2]Technical University of Darmstadt, E-mail: lang@mathematik.tu-darmstadt.de

Abstract: When working with gas transport and gas network models, one deals with multiple challenges that further complicates the approximate solution of problems in that context. Usually there are uncertainties involved, like the randomly distributed gas consumption, that can fairly quickly lead to high dimensional problems [2, 3].

In our work we are interested in optimizing on a given quantity of interest, with uncertainty involved in the constraints of the problem. These constraints should then be fulfilled with a given probability:

$$\min_{u} f(u)$$

$$\text{s.t. } P(g_i(u) \leq 0,\ i = 1, \ldots, m) \geq \alpha, \quad \alpha \in (0, 1].$$

Here we consider Kernel Density Estimation (KDE) as a technique, which allows us to approximate the uncertain optimization task with a deterministic one. That can then be tackled using established nonlinear optimization routines. The goal of KDE is to approximate the probability density function of the involved random variables, which can be challenging even for a low number of dimensions [1]. In our approach we consider a high number of inequalities, but we only use a one dimensional KDE to approximate both the success probability and the gradient with respect to the control variable u.

We demonstrate this approach in the context of gas transport to maximize technical capacities that the operator of a gas network can safely sell. Here we assume that the gas demand follows an uncertain probability distribution, hence we have to ensure that given pressure bounds are satisfied with a certain probability. We consider the isothermal Euler equations as a model with a suitable discretization to investigate the capabilities of our approach.

Keywords: Chance Constraints, Kernel Density Estimation, Stochastic Optimization, Gas Transport

---

* Presenting author

References

[1] M. Schuster, E. Strauch, M. Gugat, J. Lang. 2022. Probabilistic constrained optimization on flow networks. Optimization and Engineering 23, pp. 1-50

[2] H. Heitsch, R. Henrion, C. Tischendorf. 2024. Probabilistic maximization of time-dependent capacities in a gas network. Optimization and Engineering. https://doi.org/10.1007/s11081-024-09908-1

[3] H. Wilka, J. Lang. 2024. Adaptive hp-Polynomial Based Sparse Grid Collocation Algorithms for Piecewise Smooth Functions with Kinks. arXiv:2404.02556

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Empirically Corrected Cluster Cubature for Reduced Order Models applied to Magnetostatics

Hauke Goldbeck[1,*], **Stephan Wulfinghoff**[1]

[1]Faculty of Engineering, Kiel University, Kaiserstr. 2, 24143 Kiel, Germany (hago/swu)@tf.uni-kiel.de, https://www.tf.uni-kiel.de/matwis/cms/en

Abstract: We present a hyper-reduction technique applied to the computational homogenization in (non- linear) magnetostatics. Within the method a reduced set of integration points is identified by clustering and empirically corrected. The presented method is applied to a computationally homogenized (nonlinear) mag- netostatics model, which contains multiple phases showing different material behavior (e.g. ferromagnetic matrix with pores).

Keywords: *Computational Homogenization, Model Order Reduction, Hyper-Reduction, Magnetism*

* Presenting author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

An isogeometric collocation method for neural fields on curved geometries

NM Mohammed*, DJ Chappell and JJ Crofts

Nottingham Trent University, E-mail: neekar.mohammed@ntu.ac.uk

Abstract: The aim of this study is to develop a new numerical algorithm for simulating neural fields on curved geometries, and eventually human brain surfaces, using Computer-Aided Design (CAD) techniques. We present a CAD-integrated analysis approach, referred to as isogeometric collocation, for solving neural field equations on surfaces that closely resemble cortical geometries typically derived from neuroimaging data. Our methodology involves solving partial integro-differential equations directly using isogeometric collocation techniques, combined with efficient numerical procedures such as heat methods for determining geodesic distances between neural units. To demonstrate the effectiveness of our approach, we initially investigate localised activity patterns in a two-dimensional neural field equation posed on a torus, with the eventual goal of extending the analysis to human brain geometries derived directly from neuroimaging point cloud data. We aim to establish a comprehensive methodology that seamlessly integrates realistic geometries with the analysis of partial integro-differential equations in computational neuroscience. This study is particularly significant for two reasons. Firstly, it addresses the highly irregular nature of point clouds derived from modern neuroimaging data while mitigating the limitations of current time-consuming numerical methods. Secondly, by employing efficient geodesic computation schemes, this approach not only

models pattern formation on realistic cortical geometries but can also accommodate cortical architectures of greater physiological relevance.

Keywords: isogeometric analysis, collocation, neural fields, integro differential equations

---

* Presenting author

On Novel MPI+MPI Hybrid Techniques for Euler–Lagrange Simulations on Distributed Systems

Patrick Kopper1,∗, Anna Schwarz1, Andrea Beck1 [1]University of Stuttgart, E-mail: kopper/schwarz/beck@iag.uni-stuttgart.de

Abstract: In engineering flows with a suspended solid phase, the point-particle Euler–Lagrange method offers an enticing approach to simulate large numbers of potentially diverse particles without imposing ho- mogenization or overly strict resolution requirements. With the Euler–Lagrange method, the fluid phase is simulated with an Eulerian approach while the solid phase is represented by individual particles (or repre- sentative particle parcels) which move in a Lagrangian manner according the kinematic relation given by Newtonian mechanics. As such, the movement of the solid phase is only weakly coupled to the continuous phase and particles are allowed to freely cross cell and even partition boundaries on a distributed system.

On unstructured grids, this particle movement step requires tracking of the particle path to identify the par- ticle host element and impose potential boundary conditions. However, in classical parallelization approach using domain decomposition, geometric information is limited to the Eulerian cells associated with a given Message Passing Interface (MPI) rank. Linking the particle tracking approach to the current particle host element is not feasible on massively parallel high performance systems because particles are allowed to cross partition boundaries an arbitrary number of times. This deficiency can be addressed by constructing ghost layers or halo regions around the current Eulerian

domain, enriching the locally available computational domain with geometric information up to a certain physical distance from the domain boundaries. However, a large amount of information is duplicated by implementing a halo region on each individual MPI rank.

The present talk presents novel MPI+MPI hybrid techniques developed for Euler–Lagrange simulations on massively parallel distributed systems. Here, the high-order accurate solver for the fluid phase is provided by the Discontinuous Galerkin Spectral Element Method (DGSEM). Geometric information for both the compute node and the surrounding halo region is uniquely stored on each compute node using the MPI-3 shared memory model [1]. By combining a space-filling curve with a format for unique global indexing, any geometry information is reliably labeled, regardless of the actual domain decomposition. The combination of an efficient two-stage search algorithm with direct memory access (RDMA) and hardware offloading min- imizes initialization times. At the same time, unique global indexing enables in-memory load balancing by dynamically redistributing run time information such as field information and particle positions before seam- lessly resuming the simulation. The complete approach is publicly available under the GPL-3.0 license in the open-source Euler–Lagrange framework LEXI [2]. By presenting examples of large-scale computations of particle-laden turbulent flows on several state-of-the-art high-performance computing (HPC) systems, the framework is proven to optimize re-initialization times and scale reliably on massively parallel systems.

Keywords: high-order DG, Euler–Lagrange, high-performance computing, MPI+MPI hybrid

* Presenting author

References

[1] P. Kopper, S. Copplestone, et al. 2022. Hybrid Parallelization of Euler-Lagrange Simulations based on MPI-3 Shared Memory. Advances in Engineering Software. Vol. 174, pp. 103291.

[2] P. Kopper, A. Schwarz, et al. 2024. A framework for high-fidelity particle tracking on massively parallel systems. Computer Physics Communications. Vol. 289, pp. 108762.

A High-Order Four-Way Coupled Euler–Lagrange Approach for Particle-Laden Flow

Anna Schwarz1,*, Patrick Kopper1, Andrea Beck1 [1]University of Stuttgart, E-mail: schwarz/kopper/beck@iag.uni-stuttgart.de

Abstract: Compressible flows with suspended particles occur in a wide variety of applications, such as spray injections or aeronautical engineering. These flows typically feature complex and highly transient multiscale and multiphysics problems. As many of these applications can be categorized as dilute gas-particle flows, the common assumption is that inter-particle collisions are negligible compared to the fluid-particle interaction. While this assumption is often fulfilled when considering the average of the flow field, especially in near-wall regions, a local enhancement of the particle number density is often observed.

In this talk, we present an extension of our high-order accurate massively parallel discontinuous Galerkin spectral element framework LEXI [1] towards four-way coupled Euler–Lagrange particle- laden flow. The framework is based on the Euler–Lagrange approach, where the particles are de- scribed in Lagrangian frame of reference while the continuous phase is given in Eulerian description. Inter-particle collisions are computed exactly based on the hard-sphere approach. The framework has been previously applied to wall-resolved LES of high-Reynolds number turbulent flows with a one- and two-way coupled dispersed particulate phase, delivering accurate results while maintain- ing excellent scaling up to tens of thousands cores. This work concludes by presenting examples of large scale computations for dense particle-laden flows in complex systems and giving an outlook on the next research challenges.

Keywords: high-order DG, Euler–Lagrange, particle collisions, turbulent flow

* Presenting author

References

[1] P. Kopper, A. Schwarz, et al. 2024. A framework for high-fidelity particle tracking on massively parallel systems. CPC. Vol. 289, pp. 108762.

CM3P 2025 – Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems

1–4 July 2025, Porto, Portugal

Influence of Nitrogen Concentration on the Fracture Mechanism of Nitrogen- Doped Gamma-Graphyne Monolayer: A Molecular Dynamics Study

M.R. Dehnavi[1,a], N. Silvestre[1] ,, P. Areias [1] ,Bruno Faria[2]

[1] Department of Mechanical Engineering (DEM) IST - Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais 1, 1049-001, Lisboa, Portugal IDMEC - Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001, Lisboa, Portugal e-mail: mahmoudreza.dehnavi@tecnico.ulisboa.pt

[2] IPC-Institute for Polymers and Composites, Department of Polymer Engineering, Campus de Azurém, University of Minho, 4800-058 Guimarães, Portugal

Lithium-air batteries (LABs), with a high theoretical capacity of 3860 $mAhg^{-1}$ and sufficient redox potential (3.04 V vs. standard hydrogen electrode), are considered the next generation and future of lithium-ion batteries (LIBs). This is due to their

novel chemical redox reactions, enhanced safety, lower cost, non-toxicity, and approximately nine times higher theoretical capacity compared to traditional LIBs. However, LABs face significant challenges, such as poor cycle life and degradation during charge/discharge cycles, attributed to the loss of coulombic efficiency in the anode and cathode degradation [1]. The cathode, typically constructed from carbon allotropes, can benefit from improved chemical stability through doping processes. Gamma-graphyne [2], a novel carbon allotrope composed of single, triple, and aromatic bonds, shows promise as a material capable of enhancing capacity and gas adsorption sites for LABs. Nevertheless, its chemical resistivity needs to be improved. This enhancement can be achieved by doping nitrogen into the carbon lattice of gamma-graphyne. However, doping can alter the fracture and failure mechanisms of gamma-graphyne, and limited information exists on how these properties vary under different doping levels. In this context, the current study investigates the effects of nitrogen doping on the fracture mechanism of gamma-graphyne sheets and compares its phenomena with that of the pure material. The results reveal that increasing the percentage of nitrogen doping reduces the mechanical stability of the system and change fatigue crack propagation. Figure 1 illustrates the configurations of pure and 10% nitrogen-doped gamma-graphyne.

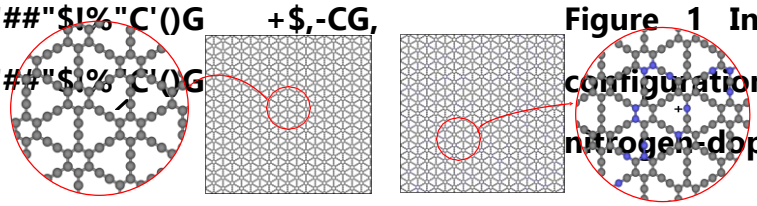


Figure 1 Intercomparison of the configurations of pure and 10% nitrogen-doped gamma- graphyne.

Keywords: Li-air batteries, Gamma-graphyne, Cathode, Doping, Nitrogen, Fracture mechanism

---

[a] Presenting Author: Mahmoudreza Dehnavi

References:

[1] Rezaee S, Araghi H, Noshad H, Zabihi Z. Physical characteristics of fluorine-doped lithium oxide as advanced material for solid- electrolyte-interphase applications of lithium–air batteries. The European Physical Journal Plus. 2022 Oct;137(10):1-6.

[2] Momen R, Rezaee R, Azizi B, Rezaee S, Hou H, Ji X. Evaluation of mechanical properties of multilayer graphyne-based structures as anode materials for lithium-ions batteries. The European Physical Journal Plus. 2022 Mar 18;137(3):360.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Physics Informed Neural Networks for coupled radiation transport equations

Laetitia LAGUZET[1,*], Gabriel TURINICI[2]

[1]CEA-DAM-DIF, F-91297 Arpajon, France, Laetitia.Laguzet@cea.fr

[2]CEREMADE, Universit´e Paris Dauphine - PSL, 75016 Paris, France, Gabriel.Turinici@dauphine.fr

Abstract:

Physics-Informed Neural Networks (PINNs) are a type of neural network designed to incorporate physical laws directly into their learning process. These networks can model and predict solutions for complex physical systems, even with limited or incomplete data, often using a mathematical formulation of a state equation supplemented with other information.

Introduced by Raissi et al. (2019), PINNs find applications in fields like physics, engineering, and fluid mechanics, particularly for solving partial differential equations (PDEs) and other dynamic systems. In this contribution we explore a modification of PINNs to multi-physics numerical simulation involving radiation transport equations; these equations describe the propagation of a Marshak-type wave in a temperature dependent opaque medium and is considered a good benchmark for difficult multi-regime computations.

The numerical simulation has to resolve a coupled system of equations : a particle transport part and a matter temperature evolution, both non-linear because of the temperature law.

Naive approaches fail in this case due to intricate relationships and a phenomena spanning several orders of magnitude; we show nevertheless that architecture changes combined with efficient boundary condition processing, time ordering sampling and adequate neural network over-parametrization treatment allow to obtain promising results.

Keywords: physics-informed neural networks; PINN, radiation transport;

---

* Presenting author

.

References

[1] Laetitia Laguzet and Gabriel Turinici. The Quantization Monte Carlo method for solving radiative transport equations. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 329:109178, 2024.

[2] Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving partial differential equations. *Journal of Computational Physics*, 378:686–707, 2019.

[3] Juan Diego Toscano, Vivek Oommen, Alan John Varghese, Zongren Zou, Nazanin Ahmadi Daryakenari, Chenxi Wu, and George Em Karniadakis. From PINNs to PIKANs: Recent advances in physics-informed machine learning, 2024.

[4] Gabriel Turinici. Optimal Time Sampling in Physics-Informed Neural Networks. In Apos- tolos Antonacopoulos, Subhasis Chaudhuri, Rama Chellappa, Cheng-Lin Liu, Saumik Bhattacharya, and Umapada Pal, editors, *Pattern Recognition*, pages 218–233, Cham, 2025. Springer Nature Switzerland.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Multi-Physical Modeling of Meta-Materials for mm-Wave Applications in the Outdoor Environment

Roshan Gomez1,∗, Michael Kaliske1 [1]Institut fu¨r Statik und Dynamic der Tragwerke (ISD),

Technische Universit¨at Dresden, E-mail: michael.kaliske@tu-dresden.de

Abstract: Meta-material devices such as the reconfigurable intelligent surface (RIS) are envisioned to be a prominent part of future wireless communication networks. Their ability to interact with electro-magnetic (EM) waves in ways not found in natural materials make them very important for future smart urban environments. Current literature on RIS and other radio-frequency meta-materials show focused engineering efforts towards the design and indoor experimental testing of RIS for mm-Wave applications [1].

A lack of outdoor testing of RIS is identified, which can be attributed to high costs of planning, frequency band licensing and the inability to control critical environmental factors. It is yet crucial to study the effects of varying environmental conditions such as temperature, moisture, wind and strains of host surface [2] on the EM response of the device. This is essential for practical deployment on existing infrastructure such as building facades. Although ray-tracing and other simulation techniques estimate the RIS-controlled EM field intensity at an abstract level, they are unable to account for the effect of other environmental factors by introducing additional fields.

It is hence proposed to develop a multi-physical finite element (FE) framework for estimating the EM field intensity towards in-silico testing of meta-materials for mm-Wave applications. Accordingly, a numerical formulation for diffraction gratings is implemented, taking into account the reconciliation of generalized refraction with diffraction theory [3]. Solution strategies to incorporate external field effects are investigated, addressing challenges due to commonly adopted assumptions in computational electro-magnetics [4] such as the harmonic time-dependence of the EM field.

Keywords: Meta-materials, finite element method, multi-physical modeling, mm-Wave

---

* Presenting author

References

[1] Ali Araghi, Mohsen Khalily, Mahmood Safaei, Amirmasood Bagheri, Vikrant Singh, Fan Wang, and Rahim Tafazolli. "Reconfigurable Intelligent Surface (RIS) in the Sub-6 GHz Band: Design, Implementation, and Real-World Demonstration". In: IEEE Access 10 (2022), pp. 2646–2655.

[2] Yan Wang, Congsi Wang, Peiyuan Lian, Song Xue, Jing Liu, Wei Gao, Yu Shi, Zhihai Wang, Kunpeng Yu, Xuelin Peng, Biao Du, and Song Xiao. "Effect of Temperature on Electromagnetic Performance of Active Phased Array Antenna". In: Electronics 9 (2020), p. 1211.

[3] St´ephane Larouche and David R. Smith. "Reconciliation of Generalized Refraction with Diffraction Theory". In: Optics Letters 37 (2012), p. 2391.

[4] Thomas Rylander, Par Ingelstr¨om, and Anders Bondeson. Computational Electromag- netics. Ed. by S. S. Antman, P. Holmes, and K. Sreenivasan. Texts in Applied Mathe- matics. New York: Springer, 2013.

Finite Element and Machine Learning-Assisted Multi-scale Simulation of Impact-Resistant Stitched Composite Shields

Masoud Mohammadi [1], Eduardo M. Sosa [2,a]

[1] West Virginia University, E-mail: mm00133@mix.wvu.edu

[2] West Virginia University, E-mail: emsosa@mail.wvu.edu

Low-velocity impacts (typically < 10 m/s) on the shell of tank cars generally used in the rail transportation industry can produce severe consequences if the impact produces hazardous materials spills. Protective stitched composite shields have been proposed to increase the puncture resistance of shells. However, the design, manufacturing, and testing of stitched composite materials for impact protection is complex and often requires multiple iterations before satisfactory results are achieved [1-2].

We present the development of a data-driven machine learning-assisted approach to simulate the impact resistance of composite shields subjected to low-velocity impacts. This research focuses on a hybrid composite manufactured with fiberglass and Kevlar fabrics stitched with Kevlar threads. The study begins by creating a multi-scale finite element (FE) simulation of the composite shield subjected to a low-velocity impact. The FE model functions across microscale, mesoscale, and macroscale scales. The FE simulation delivers peak impact force, displacements at failure, as well as the level of energy absorption. The FE results are then utilized to train artificial neural networks (ANNs). To generate training data, the FE simulations are automated with scripts created to manage

multiple simulations, systematizing data outputs to create a large dataset for analyzing the composite under a range of low-velocity impacts at both the mesoscale and macroscale levels.

The FE data then trains ANNs at each scale, coupled to form a multi-scale machine learning-assisted simulation. The mesoscale ANN uses homogenized mechanical properties (HMPs) from the microscale model of the composite layers to predict mesoscale HMPs where a combination of layers and stitching threads are considered in a mesoscale representative

[a] Presenting Author

References:

[1] M. Mohammadi. 2024. Machine learning-assisted multiscale simulation and design optimization of composite jackets under low-velocity impacts. West Virginia University Graduate Theses, Dissertations, and Problem Reports, 12661.

[2] M. Mohammadi, E.M. Sosa. 2024. Enhancing mode-II delamination resistance of hybrid woven composite materials of glass/Kevlar fabrics by stitching with Kevlar threads. Composite Structures 2024;345:118365.volume element. The macroscale ANN then uses the mesoscale HMPs to produce the composite's impact response.

The multi-scale ANN system is also integrated with a particle swarm optimization algorithm adopted to explore the design space and find the optimal composite configuration for specific impact conditions and constraints. All FE simulation results and predictions from the multi-scale ANN are validated against experimental data on composites subjected to low- velocity impacts.

The proposed multi-scale ANN approach presented in this study is flexible. It has the potential for being implemented in other complex materials and structures where multiple variables across different scales could change the outcome and where several possible combinations of the design space need to be evaluated to find the optimal combination for a given set of constraints, but only taking a small fraction of the time that multiple FE simulations would take to compute.

Keywords: Multi-scale Simulation, FEM, Machine Learning, Stitched Composite.CM3P 2025 - Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Coupling incompressible Newtonian fluids, visco-elastic fluids, and elastic solids: an Eulerian model for multiphase flows

Alexandre Caboussat[1,*], L´eo Diserens[1,2], Marco Picasso[2]

[1] Geneva School of Business Administration (HEG-Gen`eve), University of Applied Sciences and Arts Western Switzerland (HES-SO), alexandre.caboussat@hesge.ch, leo.diserens@hesge.ch

[2] Institute of Mathematics, Ecole polytechnique f´ed´erale de Lausanne, 1015 Lausanne, Switzerland, marco.picasso@epfl.ch, leo.diserens@epfl.ch

Abstract:

We present a numerical model for the simulation of multiphase flows with multiple rheologies. The model allows to incorporate in a unified manner several phases ranging from incompressible Newtonian flows, Oldroyd-B viscoelastic flows, and neo-Hookean elastic solids.

Computational solid mechanics are usually formulated in Lagrangian variables, the displacement being the unknown, whereas computational fluid mechanics are formulated

in Eulerian variables, the velocity being the unknown. Moreover, the partial differential system arising from solid mechanics is of hyperbolic type, whereas partial differential equations arising from fluids are of parabolic type. Hence it is usually difficult to solve numerically problems involving fluids and deformable solids, due to these various behaviors and the underlying multiple time scales.

We propose an Eulerian model for mutiphase flows that uses a common mathematical formulation for all phases, and is inserted into a unique numerical method. The formulation of the model for elastic solids is a straightforward extension of that for an Oldroyd-B viscoelastic fluid. While being surprisingly simple, it allows to account for large deformations of elastic solids, and changes of topologies.

We rely on a volume tracking approach based on the individual volume fractions of liquid of each phase, and a volume-of-fluid method. The numerical framework relies on an operator splitting strategy for the time discretization to decouple advection and diffusion operators. A two-grid method is advocated for the space discretization, with a fine structured Cartesian grid, and a coarser unstructured finite element mesh.

Numerical experiments are presented to validate the mathematical model, by addressing several configura- tions involving all types of rheologies. We discuss for instance the interactions between two elastic bodies, or between elastic bodies and visco-elastic fluids, for instance to absorb shocks.

Keywords: Multiphase flows, multiple rheologies, visco-elastic fluids, Neo-Hookean elastic solids, large deformations, unified model, operator splitting, two-grid method,

* Presenting author

References

[1] M. Picasso. 2016. From the free surface flow of a viscoelastic fluid towards the elastic deformation of a solid. Comptes Rendus Math´ematique, Vol 354(5), pp 543–548.

[2] L. Diserens. 2023. Numerical simulation of immiscible incompressible viscous, viscoelas- tic and elastic multiphase flows. PhD thesis, EPFL.

Modeling of Air Purification Processes Using Multilayer Porous and Sorbent Filters

KUDRYASHOVA T. A. [1,a], POLYAKOV S. V. [2], TARASOV N. I. [3]

[1] Keldysh Institute of Applied Mathematics, RAS, E-mail: kudryashova@imamod.ru

[2] Keldysh Institute of Applied Mathematics, RAS, E-mail: polyakov@imamod.ru

[3] Keldysh Institute of Applied Mathematics, RAS: nikita_tarasov@imamod.ru

Air purification from pollutants is a topical issue for many industrial technologies and quality of life environment. In this challenge, the most relevant are new methods of purification from polydisperse solid nanoparticles. These particles pose the greatest danger to humans and other living organisms. The solution of this environmental problem requires comprehensive studies of pollution processes and, accordingly, purification of the air environment from such pollutants. At present, the most effective way to study pollution and purification processes is computer modeling.

In this work, we have chosen the task of cleaning the air environment from solid nano-sized impurities of various types with the use multilayer porous and sorbent filters. In the first approximation, a multilayer filter system can be considered as a single object with variable porosity. Under these assumptions, we have developed an end-to-end mathematical model (it means that free flow and flow in a porous medium are considered simultaneously) of a treatment system in 3D geometry, based on a macroscopic quasi-gasdynamic approach [1]. The model allows us to calculate the air flow in the space in front of, inside and behind the porous filter. The main cleaning processes are modeled in the filter area using convection-diffusion type equations written relative to the concentrations of polluting particles [2]. In this case, nanoparticles are divided into two classes – charged and neutral, and also by composition. To solve such a mathematical problem, a finite volume grid method has

been developed [2, 3], supplemented by special numerical models of nanoparticle adsorption on the internal boundaries of a porous body. The general numerical algorithm is implemented by software with parallel technologies.

Using the developed software tools, a series of numerical experiments on air purification from household and coal dust were conducted. They confirmed the correctness of the developed mathematical model and the effectiveness of its computer implementation. In addition, the results of the numerical experiments make it possible to apply the developed methodology in the design of new filtration devices and their subsequent efficient operation.

Keywords: air purification, mathematical models, numerical methods, ecology, filtration, multilayer porous filters.

References:

[1] *Elizarova T.G.* Quasi-Gas Dynamic Equations. Springer-Verlag: Berlin, Heidelberg, 2009. 286 p.

[2] S.V. Polyakov, Yu.N. Karamzin, T.A. Kudryashova, V.O. Podryga, D.V. Puzyrkov,

N.I. Tarasov. Multiscale supercomputer modeling of gas purification processes by adsorption.

---

[a] Presenting Author

// Computational methods and programming. 2020. V. 21. P. 64-77. https://doi.org/10.26089/NumMet.v21r106

[3] *Yuri N. Karamzin, Tatiana A. Kudryashova, Sergey V. Polyakov.* On a class of flux schemes for convection-diffusion equations // Computational Mathematics and Information Technologies, 2017, vol. 1, No. 2, pp. 169-179

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Phase-field modeling of initiation and propagation of cracks in heterogeneous porous solids due to thermal effects

Ze-chao Chen[1,*], Laura De Lorenzis [2], Lorenzo Sanavia[3]

[1]Center of Studies and Activities for Space (CISAS) - "G. Colombo", University of Padova, E-mail: zechao.chen@phd.unipd.it

[2]Department of Mechanical and Process Engineering Eidgenossische Technische Hochschule Zurich, Zu¨rich, Switzerland, E-mail: ldelorenzis@ethz.ch

[3]Department of Civil Environmental Architectural Engineering, University of Padua, Padova, Italy, E-mail: lorenzo.sanavia@unipd.it

Abstract:

Phase-field modeling has been widely recognized as an effective framework for predicting the initiation and evolution of drying cracks in variably saturated porous media[1-5]. The presented work aims at the develop- ment and validation of a general thermo-hydro-mechanical phase-field model able to study the nucleation and propagation of cracks induced by thermo-hydro-mechanical effects in multiphase porous materials. Based on the earlier research ([1], [2], [3]), the new model can describe cracking in variably saturated deformable porous media taking into account heat flow, flows of liquid water and gas and water evaporation/condensation.

The model capabilities are validated by simulating several examples, including mechanical, hydro-mechanical and thermo-hydro-mechanical cracks. The developed model highlights the influence of thermal effects on crack initiation and propagation, and provides insights into the complex interplay between drying, desatu- ration, and fracture mechanics in porous media.

Keywords: Phase-field fracture, Thermo-hydro-mechanical coupled problems, Finite element method.

---

* Presenting author

References

[1] Cajuhi T., L. Sanavia, L. De Lorenzis, Phase-field modeling of fracture in variably saturated porous media. Computational Mechanics 61 (2018), 299-318.

[2] Gavagnin C., L. Sanavia, L. De Lorenzis, Stabilized mixed formulation for phase-field computation of deviatoric fracture in elastic and poroelastic materials. Computational Mechanics 65 (2020), 1447–1465.

[3] Luo, C., Sanavia, L., De Lorenzis, L. Phase-field modeling of drying-induced cracks: Choice of coupling and study of homogeneous and localized damage. Computer Methods in Applied Mechanics and Engineering, 410 (2023), 115962.

[4] Heider Y., W. Sun, A phase field framework for capillary-induced fracture in unsaturated porous media: Drying-induced vs. hydraulic cracking, Comput. methods Appl. Mech. Engrg. 359 (2020), 112647.

[5] Cheng, Panpan, et al. "Coupled thermo-hydro-mechanical-phase field modeling for fire- induced spalling in concrete." Computer Methods in Applied Mechanics and Engineering 389 (2022), 114327.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Multiscale and Multiphysics Framework for Thermal and Structural Analysis of Load-Bearing Heat Exchangers in Sustainable Aircraft

Girindra Ramgobin [1,*], Harvey M. Thompson[2], Amirul Khan[3], Martin Muir[4], Gregory N. de Boer[2]

[1] EPSRC Centre for Doctoral Training in Fluid Dynamics, University of Leeds , E-mail: scgr@leeds.ac.uk

[2] School of Mechanical Engineering, University of Leeds

[3] School of Civil Engineering, University of Leeds

[4] Airbus Central Research and Technology, Filton, Bristol, UK

Abstract: The shift towards sustainable aviation, driven by alternative propulsion systems powered by liquid hydrogen and batteries, calls for innovative thermal management solutions. These propulsion systems release significant low-grade heat that must be efficiently dissipated by heat exchangers (HX) to ensure op- erational safety and performance. Moreoever, with energy storage shifting from traditional wing-mounted fuel tanks to batteries or cryogenic tanks in the fuselage, the wings are largely unoccupied. While this alleviates volumetric constraints, it introduces new structural challenges, such as managing wing bending. Incorporating HX into the wings presents an opportunity to enhance aero-structural stiffness by enabling them to serve as load-bearing components. This introduces a complex multidisciplinary problem involving thermal, structural, and aerodynamic performance. By leveraging a combined multidisciplinary analysis for the design of these HX, there is a substantial opportunity to reduce weight and improve the aerodynamic performance of these sustainable aircraft.

The integration of multiscale and multiphysics methods into an optimisation study, as recently demon- strated by Tancabel et al. [1], highlights the growing relevance of this combined approach for HX. While numerous multiscale studies have explored cross-flow HX, variations in microscale geometries and upscaling techniques—ranging from thermally developing boundary flow models to surrogate models—are prevalent. To address this challenge and investigate the selection of microscale geometries, we present a novel multi-scale and multiphysics modular framework for cross-flow HX. The framework's first module investigates the thermal performance of microscale geometries, as shown in Figure 1, expanding on an established multiscale method by Ciuffini et al. [2]. Various microscale domains—ranging from single unit cells to clustered cells, channels, and layers—are benchmarked against a full-scale conjugate heat transfer model of the HX. Metrics such as pressure loss and local heat transfer coefficients are compared to validate the framework's accuracy and computational efficiency. On the structural side, unit cell characterisation involves applying uniaxial and shear loads to derive the stiffness matrix and evaluate the structural response. Once preliminary ther- mal and structural assessments meet performance requirements, the framework advances to high-fidelity aerothermal-structural simulations that incorporate thermal stresses, enabling a detailed analysis of the combined effects of thermal and mechanical loads. Future work will involve integrating this framework into a surrogate model-based multidisciplinary optimisation study, as shown in Figure 2, followed by a mission profile analysis for sustainable aircraft. This will enable a comprehensive evaluation and optimisation of HX integration within the broader thermal management system, across the entire flight envelope.

Keywords: Heat Exchangers, Multiscale, Multiphysics

---

* Presenting author

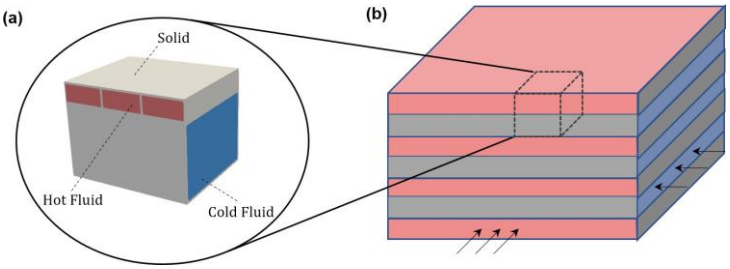


Figure 1: Diagram showing (a) the microscale unit cell geometry of the cross flow HX and (b) the macroscale domain. Arrows represent direction of fluid flow.

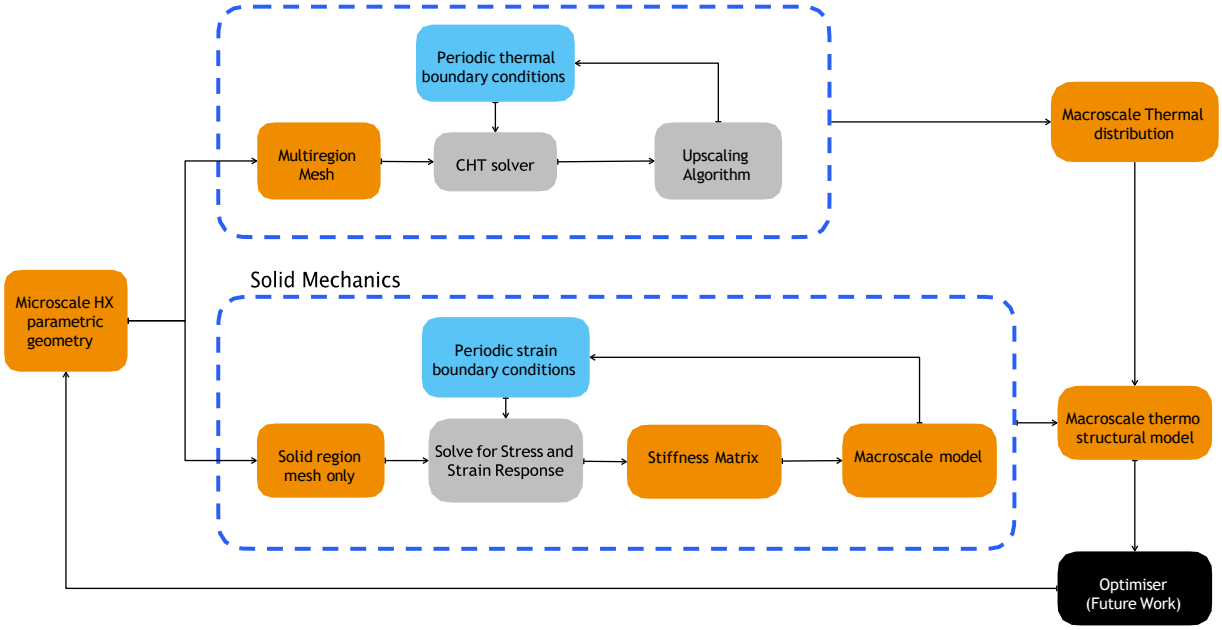


Figure 2: Workflow for the thermal and structural multi-scale analysis of the heat exchanger. All simulations carried out in OpenFOAM and data processing performed in python.

.

References

[1] J. Tancabel et al., "Multi-scale and multi-physics analysis, design optimization, and experimental validation of heat exchangers utilizing high performance, non- round tubes," Applied Thermal Engineering, vol. 216, p. 118965, Nov. 2022, doi: 10.1016/j.applthermaleng.2022.118965.

[2] A. Ciuffni, A. Scattina, F. Carena, M. Roberti, G. Toscano Rivalta, E. Chiavazzo, M. Fasano, and P. Asinari, "Multiscale computational fluid dynamics method- ology for predicting thermal performance of compact heat exchangers," Jour- nal of Heat Transfer, vol. 138, no. 7, p.071801, Jul. 2016. [Online]. Available: https://asmedigitalcollection.asme.org/heattransfer/article/doi/10.1115/1.4032980/375424/Multiscale-Computational-Fluid-Dynamics

Unravelling the Interplay between Mesh-Dependent Effects Across Spatial Scales with Second-Order Computational Homogenisation

Guilherme Fonseca Gonçalves[1,a], Igor A. Rodrigues Lopes[2], Francisco M. Andrade Pires[1,2]

[1] FEUP, Faculdade de Engenharia da Universidade do Porto, Department of Mechanical Engineering, E-mail: up201907304@up.pt, fpires@fe.up.pt

[2] INEGI-LAETA, Instituto de Ciência e Inovação em Engenharia Mecânica e Engenharia Industrial, Universidade do Porto, E-mail: ilopes@fe.up.pt

Employing multi-scale models based on computational homogenisation to examine the failure of structures and components remains a challenging endeavor since strain localisation and softening lead to mesh-dependent effects across spatial scales. This study investigates the attenuation of mesh-dependency in multi-scale computational-homogenisation-based models, including the role of the RVE (Representative Volume Element) length and the combined effects of micro- and macro-scale softening. To that end, two numerical examples of multi-scale strain softening are presented, considering porous RVEs to mimic the failure mechanisms of ductile materials. A constitutive model for finite strain elastoplasticity is adopted, together with a simple damage evolution law.

Second-order homogenisation reduces macro mesh-dependency and prevents spurious deformations, due to the introduction of a macroscopic intrinsic length-scale. This length-scale is intimately related to the RVE length and evolves throughout the deformation path. Its role in the resulting second-order multi-scale predictions is carefully assessed. The bounds for utilising the RVE length as a numerical parameter controlling macro-scale localisation and softening are analysed. Moreover, the second-order multi-scale

formulation considered in this contribution does not tackle RVE mesh-dependency, which persists due to microscopic softening sources. The impact of micro-scale softening is examined by adopting a nonlocal damage model, yielding an important reduction in RVE mesh-dependency. Attenuating micro mesh-dependency increases the effectiveness of macro-scale regularisation. These findings demonstrate the intricate interplay between mesh-dependent effects at both scales, particularly in the presence of strong localisation.

Keywords: Multi-scale models based on computational homogenisation; second-order computational homogenisation; strain softening and localisation; Mesh-dependency

---

[a] Presenting AuthorCM3P 2025 - Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems

2–4 July 2025, Porto, Portugal

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Numerical study of deflagration in small compartment employing finite rate chemistry mechanisms

Marcos Vanella[a*], Chandan Paul[a,b], Thomas Cleary[a], Ryan Falkenstein-Smith[a]

[a]National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, USA

[b]The George Washington University, 800 22nd Street, NW, Washington DC, USA

[*]Corresponding author : marcos.vanella@nist.gov

Abstract: In fires in the built environment, backdraft deflagrations pose a great risk to occupants and first responders. The phenomenon involves a vitiated atmosphere in a closed compartment containing a rich mixture of gaseous fuels, products and air. If the compartment is by some means opened to the exterior, a cold air current is introduced inducing a variation in mixture composition which can lead to flammable conditions. Further, if a hot surface or ember is present in this location, ignition and violent deflagration can result. Understanding conditions conducive to ignition and flame propagation in this context is essential for backdraft risk reduction.

Several studies are found in the literature on the simulation of such transient scenario, i.e. [1, 2]. In particular, our target scenario varying gaseous fuel loads is based on backdraft experiments in a scaled compartment recently performed at the National Institute of Standards and Technology (NIST) [3]. In these experiments spark-ignitors were employed to trigger deflagration in a 1.5 m long by 1 m wide by 1 m height compartment after its door was opened. For propane fuel experiments, the mass flow rate and fuel flow time (FFT)

in a sand burner in the back of the compartment was varied to set the amount of unburnt fuel and resulting deflagration propensity.

In our efforts employing the Fire Dynamics Simulator (FDS) [4], we have evaluated the use of default mixing controlled fast chemistry to simulate this problem [5]. Three main challenges make this approach undesirable: the need to define heuristic extinction and ignition models, and FDS not being designed to perform large eddy simulation (LES) for partially premixed combustion. In particular, the use of a temperature ignition threshold to allow combustion to proceed makes simulated deflagration outcomes highly dependent on the LES grid size. For the range of grid sizes studied, using the default fuel auto ignition temperature as ignition threshold would preclude deflagration to occur even in high fuel load cases where backdraft was invariably seen in experiments.

On the other hand, utilizing finite-rate chemistry, either through two or three step global mechanisms or skeletal detailed chemistry mechanisms, enables more accurate modeling of ignition and extinction without relying on heuristic models. However, this requires direct numerical simulation (DNS) level grid resolution to capture correct temperatures and flame thickness, or special treatment to account for unresolved turbulence and chemistry interaction in LES models. Moreover, to accurately capture flame propagation in our problem, finite-rate combustion mechanisms must be validated to ensure they exhibit correct physical behavior. For instance, the selected mechanism should accurately predict laminar flame speeds across a range of equivalence ratios.

In this work the focus will be on employing finite-rate kinetics in a coupled approach to simulate backdraft events in the NIST scaled compartment. The objective is to address key questions: How detailed must the chemical mechanism be to accurately predict ignition, extinction, and flame propagation? What level of domain resolution is required to reasonably match experimental observations of backdraft and flame propagation? Finally, how does the initial compartment composition influence the backdraft event? To achieve this, we propose the following:

- We will simulate the flame propagation characteristics of the two-step Westbrook and Dryer [6] and Jones-Lindstedt [7] global chemical mechanisms for propane in two-dimensional computations within FDS. Additionally, we will examine the behavior of the relatively small Z66 detailed mechanism [8], which consists of 24 species and 66 reactions. The results, particularly the flame speed at different equivalence ratios, will be compared with flame speed calculations obtained using the same mecha- nisms in the Cantera software package [9], validating FDS's implementation of detailed chemistry. We will also determine the grid resolution required to accurately capture flame propagation.
- Use experimental results to define the initial temperature and gas mixture conditions [10] for two extreme scenarios in which a 25 kW propane burner was employed. The first scenario involves an FFT of 210 s, where backdraft was never observed, while the second scenario, with an FFT of 300 s and a higher fuel load, consistently resulted in deflagration. Simulations of deflagration will then be

performed for these initial conditions using both the two-step global chemical mechanisms and the detailed chemical mechanisms. The outcomes of the resulting deflagration events will be compared with experimental results.

Keywords: Fire Simulation, Detailed Chemistry, Combustion, Backdraft.

---

* Presenting author

References

[1] WG Weng, WC Fan, and Y Hasemi. Prediction of the formation of backdraft in a compartment based on large eddy simulation. *Engineering Computations*, 22(4):376–392, 2005.

[2] SA Ferraris, JX Wen, and S Dembele. Large eddy simulation of the backdraft phenomenon. *Fire Safety Journal*, 43(3):205–225, 2008.

[3] R Falkenstein-Smith and T Cleary. Thermal and gas mixture composition measurements preceding backdrafts in a 2/5th scale compartment. NIST Technical Note 2185, National Institute of Standards and Technology, 2022.

[4] K. McGrattan, S. Hostikka, R. McDermott, J. Floyd, C. Weinschenk, and K. Overholt. *Fire Dynamics Simulator, User's Guide*. National Institute of Standards and Technology,

Gaithersburg, Maryland, USA, and VTT Technical Research Centre of Finland, Espoo, Finland, sixth edition, September 2013.

[5] Marcos Vanella, Ryan Falkenstein-Smith, and Thomas Cleary. Backdraft experiments and large eddy simulations in a scaled compartment. *Fire Safety Journal*, 141:103960, 2023.

[6] Charles K. Westbrook and Frederick L. Dryer. Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames. *Combustion Science and Technology*, 27:31–43, 1981.

[7] W.P. Jones and R.P. Lindstedt. Global reaction schemes for hydrocarbon combustion. *Combustion and Flame*, 73(3):233–249, 1988.

[8] N. Zettervall, K. Nordin-Bates, E.J.K. Nilsson, and C. Fureby. Large eddy simulation of a premixed bluff body stabilized flame using global and skeletal reaction mechanisms. *Combustion and Flame*, 179:1–22, 2017.

[9] David G. Goodwin, Harry K. Moffat, Ingmar Schoegl, Raymond L.Speth, and Bryan W. Weber. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. https://www.cantera.org, 2023. Version 3.0.0.

[10] Marcos Vanella, Chandan Paul, Ryan Falkenstein-Smith, and Thomas Cleary. A study on local conditions conducive to deflagration in a scaled compartment. G-3 Enclosure Fire Dynamics. 13th Asia-Oceania Symposium on Fire Science and Technology AOSFST, October 22-24, 2024, Daegu, Republic of Korea.

Chebyshev collocation method for the stability of ferromagnetohydrodynamic Poiseuille blood flow incorporating micromagnetorotation

Kyriaki-Evangelia Aslani 1,a, Ioannis E. Sarris 2, Efstratios Tzirtzilakis 1 [1]
Department of Mechanical Engineering, University of the Peloponnese, k.aslani@go.uop.gr; etzirtzilakis@uop.gr.

[2] Department of Mechanical Engineering, University of West Attica, sarris@uniwa.gr.

A micropolar fluid is defined as any fluid that contains small, rigid particles that move autonomously within the fluid. The theory of micropolar fluids was developed by Eringen in 1966 and constitutes an extension of the Navier-Stokes equations used to describe Newtonian fluids. Micropolar fluid theory differs from Navier-Stokes equations due to the presence of the antisymmetric part of the stress tensor, which is zero in the latter. The antisymmetric part of the stress tensor contributes to the equation for the conservation of angular momentum, which is not satisfied identically as in the Navier- Stokes equations. Thus, in micropolar fluids, another equation needs to be solved, i.e., the equation of the change of the internal angular momentum. Based on all this, a micropolar fluid is described not only by its axial velocity, but also by its microrotation $\boldsymbol{\omega}$. The micropolar fluid theory has found application in the modelling of a variety of fluids, such as exotic lubricants, colloidal suspensions, liquid crystals, and blood [1].

An important class of micropolar fluids is the ferrofluids, which consist of ferromagnetic nanoparticles (such as magnetite) into a mother-liquid carrier (such as water or kerosene). Ferrofluids can have applications in both engineering and biomedicine, mainly because of their rheological properties that can be easily controlled by an externally applied magnetic field. A key characteristic of ferrofluids is the magnetic polarization of the particles (magnetization) $\boldsymbol{M}$, which tends to 'relax'

and align with the external magnetic field $\boldsymbol{H}$. This creates a magnetic moment $\boldsymbol{M} \times \boldsymbol{H}$ that contributes to the equation of change of the internal angular momentum and can significantly affect the microrotation of the ferromagnetic nanoparticles in the fluid. This phenomenon was extensively studied by Shizawa & Tanahashi [2], who presented a complete mathematical model for ferrofluids using the micropolar fluid theory and Maxwell's equations while introducing a new equation for the magnetization change taking into account the existing microrotation of the ferromagnetic nanoparticles (micromagnetorotation-MMR).

As mentioned above, blood is classified as a micropolar fluid, due to the existence of the blood cells in the plasma. Moreover, some studies suggest that blood should be treated as a ferrofluid under an external applied magnetic field (for example when a magnetic resonance image-MRI scanner is used). Blood contains the hemoglobin molecule in the erythrocytes (red blood cells), which is an iron oxide and behaves like a magnetic particle, while blood plasma is the mother-liquid carrier [3]. Consequently, the applied magnetic field may influence the microrotation of the erythrocytes due to the magnetization of hemoglobin, subsequently impacting blood viscosity and velocity. There are experimental studies that provide statistically significant evidence of symptoms, such as vertigo, nausea, and metallic taste for magnetic field intensities of 1.5 and 4T associated with blood velocity reduction [4]. Furthermore, these observations cannot be attributed to the Lorentz force's impact on the

[a] Presenting Author

blood flow, as the small electrical conductivity of blood prevents it from being influenced by the Lorentz force [3].

Recently, Aslani et al. [5-7] made several analytical studies on the impact of micromagnetorotation on micropolar magnetohydrodynamic (MHD) flows (such as blood) using the mathematical model of Shizawa and Tanahashi. These studies focused on establishing the differences arising by acknowledging and ignoring the MMR term, while the effect of the Lorentz force was always included. It has been shown that when the effect of the MMR was included, deceleration of the flow was up to 16%, whereas microrotation reduction was up to 99%. It has been proved that an externally applied magnetic field on a blood flow affects erythrocytes' microrotation through the MMR term, which in turn affects blood's velocity, a phenomenon mentioned in many experimental studies that cannot be explained only by the effect of the Lorentz force.

Considering all the above, this research focuses on the investigation of the stability of an MHD micropolar blood Poiseuille flow by acknowledging the effect of micromagnetorotation. After the analytical solution of the governing equations (i.e. the model of Shizawa and Tanahashi for micropolar ferrofluid flows), a modified sixth-order Orr-Sommerfeld equation is derived for the first time, which incorporates the micropolar nature of blood, the effect of the Lorentz force and the micromagnetorotation. The manipulation of the latter leads to an eigenvalue problem which is solved using a numerical code based on the free open-source software "Chebfun" and "Chebop" in MATLAB [9]. This code utilizes the Chebyshev collocation method and has been previously used for the solution of the classical Orr-Sommerfeld equation. It was found that the both Lorentz force and the MMR

term have a strong stabilizing effect on the MHD micropolar blood flow. The effect of the MMR is more intense than that of the Lorentz force. Thus, the MMR is proved to be a mechanism that dissipates magnetic energy to the blood flow via erythrocytes' microrotation. The results of this study are anticipated to be of great value for bioengineering applications that involve magnetic fields applied to blood flows (such as magnetic hyperthermia and magnetic drug delivery).

Keywords: micropolar fluid; blood; ferromagnetohydrodynamics; magnetization; stability analysis; Chebyshev collocation method.

References:

[1] G. Lukaszewicz. 1999. Micropolar fluids: theory and applications. Springer Science & Business Media.

[2] K. Shizawa, T. Tanahashi. 1986. New constitutive equations for conducting magnetic fluids with internal rotation: Thermodynamical discussions. Bull. JSME, Vol. 29, pp. 2878-2884.

[3] E. Tzirtzilakis. 2005. A mathematical model for blood flow in magnetic field. Phys. Fluids, vol. 17, p. 077103.

[4] J. F. Schenck, C. Dumoulin, R. Redington, H. Kressel, R. Elliott, I. McDougall. 1992. Human exposure to 4.0-Tesla magnetic fields in a whole-body scanner. Med. Phys., Vol. 19, pp. 1089-1098.

[5] K.-E. Aslani, E. Tzirtzilakis, I. E. Sarris. 2024. On the mechanics of conducting micropolar fluids with magnetic particles: Vorticity–microrotation difference. Phys. Fluids, Vol. 36, p. 10.

[6] K.-E. Aslani, I. E. Sarris. 2021. Effect of micromagnetorotation on magnetohydrodynamic Poiseuille micropolar flow: Analytical solutions and stability analysis. J. Fluid Mech., Vol. 920, p. A25.

[7] K.-E. Aslani, I. E. Sarris. 2021. Effect of micromagnetorotation on the heat transfer of micropolar Hartmann flow. Therm. Sci. Eng. Prog., Vol. 26, p. 101129.

[8] Z. Battles, L. N. Trefethen. 2004. An extension of MATLAB to continuous functions and operators. SIAM

J. Sci. Comput., Vol. 25, pp. 1743-1770

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Numerical Assessment of Insulation System Design for 20 CBM Liquefied Hydrogen Tank using Concept of Cryogenic Sacrificial Fluid Shielding

Gun Woo Kim [1,a], Ha-yeong Kim[1], Dong Hee Hong[1], Hyun-seok Kim [1]

[1] Korea Research Institute of Ships and Ocean Engineering

Corresponding Author E-mail: gwkim@kriso.re.kr

In this study, the performance evaluation of the insulation system using cryogenic sacrificial fluid shielding for liquefied hydrogen storage was conducted numerically. As the demand for eco-friendly energy systems increases worldwide, research on hydrogen energy systems is receiving great attention in the ships and ocean engineering. However, the commercialization is delayed due to the small energy density per volume of hydrogen. To solve this problem, many groups are researching liquid hydrogen. Liquid hydrogen, made by cooling hydrogen to cryogenic temperature of -253°C, can have a density twice that of gas hydrogen. In general, high-vacuum MLI insulation technology is applied to the insulation system of the storage. But in the sector of ships and maritime, it is difficult to maintain high-vacuum insulation due to the characteristics of large scale and a rough ocean wave environment. To overcome disadvantage, the design of the cryogenic sacrificial fluid shielding insulation system applicable to ships and ocean sectors was conducted in this study. The cryogenic sacrificial fluid is a substitute that protects the liquid

hydrogen by absorbing penetrating heat and vaporizing it on its own. Various cryogenic fluids were evaluated as cryogenic sacrificial fluids, the already proven medium vacuum (50 mtorr) perlite insulation was used considering application to ship, and the designed insulation system was applied to the 20 CBM liquefied hydrogen storage. Finally, the performance of developed insulation system was evaluated using CFD analysis techniques. As a result, it was confirmed that the penetration heat was reduced by 56.7% compared to the simple Perlite insulated vessel.

Keywords: Liquefied Hydrogen Storage Tank, Insulation System, Cryogenic Sacrificial Fluid Shielding, Computational Fluid Dynamics (CFD)

Acknowledgement: This research was supported by the grant from National R&D Project "Research Hub Establishment and International Joint Research on Advanced Maritime Mobility (AMM) between Korea and Europe" funded by Ministry of Oceans and Fisheries (RS-2024- 0041020).

a Presenting Author, Corresponding Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Novel Concept Design for Efficient Storage and Carriage of On-board Captured CO2: Mid-ship Shaped Vertical Tri-Lobe LCO2 Tank

Jin-Ho Lee [1,2,a], Ha-Yeong Kim[3], Hyun-Seok Kim [4, b]

[1] University of Science and Technology, E-mail: ljh0714@kriso.re.kr

[2] Korea Research Institute of Ships & Ocean Engineering, E-mail: ljh0714@kriso.re.kr

[3] Korea Research Institute of Ships & Ocean Engineering, E-mail: hykim08@kriso.re.kr

[4] Korea Research Institute of Ships & Ocean Engineering, E-mail: hskim85@kriso.re.kr

Recently, the International Maritime Organization (IMO) established its revised strategy to achieve net-zero emissions around 2050. Attaining carbon neutrality requires collaboration and share of experience regarding alternative eco-friendly fuels among multidisciplinary. Although, adopting carbon-free fuels might seem promising, yet readiness of infrastructures and availability are far to reach economic feasibility, usage of fossil fuels is inevitable for ships. Therefore, on-board CCS (Carbon Capture and Storage) technologies has gathered significant attention within the organization and, also the members as feasible solution to achieve carbon neutrality while securing economic. In particular, the liquefaction method for efficiently transporting emissive carbon dioxide is emerging as a key technology. However, storage and transportation of LCO2 (Liquefied Carbon Dioxide) is not an easy task for ships, as they have to take into account their weight, stability of the vessel, visibility due to tank height, etc. Also, LCO2 requires

high-pressure storage. Thus, membrane-type storage is not feasible, making type C tank is the most reasonable choice.

This study proposes a new design for a vertical tri-lobe tank, aimed at maximizing space utilization and improving the transport efficiency of LCO2. This study considers two different types of ship as case study which is the VLCC (Very Large Crude oil Carrier) and LNGC (Liquefied Natural Gas Carrier). The research considers the cross-sectional area of the target ship's cargo holds used for carbon capture storage to calculate its storage capacity. Furthermore, a comparative analysis is performed with existing design of type C tank and bi- lobe tank to evaluate the space optimization validity.

First, the conceptual design was carried out by considering the static and dynamic pressures and acceleration of the tank following the IGC (International Code of the Construction and Equipment of Ships Carrying Liquefied Gases in Bulk) code and ASME (American Society of Mechanical Engineers) code. The study also performed a scantling calculation of the proposed vertical tri-lobe tank design in accordance with Classification Society's Rules. Structural safety was verified by identifying the maximum stress and displacement points through structural analysis using the ANSYS software. After that, the validity of using the vertical tri-lobe tank was verified by comparing the storage capacity and space efficiency through comparison between the designed vertical tri-lobe tank and the existing type C tank, bi-lobe tank.

The results demonstrate the potential to enhance the efficiency of maritime storage and

[a] Presenting Author, [b] Corresponding Author

transportation of LCO2 while providing a technical foundation for achieving carbon neutrality. The proposed vertical tri-lobe tank represents a significant technical advancement, offering a safe and efficient solution for future LCO2 transport and contributing to the transition toward a carbon-neutral society.

Keywords: LCO2 (Liquefied Carbon Dioxide), On-board CCS (Carbon Capture and Storage), Tri-Lobe Tank, Space Efficiency, Structure Analysis

Acknowledgement: This research was supported by Korea Research Institute of Ships and Ocean engineering a grant from Endowment Project of "Technology Development of Onboard Carbon Capture and Storage System and Pilot Test" funded by the Ministry of Oceans and Fisheries, Korea(2520000280/PES5482).

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Innovative Designs for Liquefied Hydrogen Fuel Storage Tank in Ships

Hyun-Seok Kim[1,a], Gun Woo Kim[2], Dong Hee Hong [3], Jae-Hwan Jung[4], Byoungjae Park[5]

[1] Korea Research Institute of Ships and Ocean Engineering(KRISO), E-mail: hskim85@kriso.re.kr

[2] Korea Research Institute of Ships and Ocean Engineering(KRISO), E-mail: gwkim@kriso.re.kr

[3] Korea Research Institute of Ships and Ocean Engineering(KRISO), E-mail: davis.hong@kriso.re.kr

[4] Korea Research Institute of Ships and Ocean Engineering(KRISO), E-mail: jaehwan@kriso.re.kr

[5] Korea Research Institute of Ships and Ocean Engineering(KRISO), E-mail: byoungjae@kriso.re.kr

Hydrogen is emerging as a promising alternative fuel for carbon-neutral shipping, yet its low volumetric energy density necessitates efficient liquefied storage solutions. This study presents the development of an IMO Type C liquefied hydrogen (LH2) fuel storage tank tailored for coastal ships, focusing on enhanced thermal efficiency and practical shipboard application.

Three innovative designs were introduced to improve tank performance. First, a topology-optimized support structure between the inner and outer tanks was developed to minimize thermal conduction while maintaining structural integrity under ship motion-induced loads. Second, a specialized baffle system was designed to mitigate sloshing effects, reducing impact forces and preventing

excessive heat transfer that could lead to uncontrolled vaporization. Third, a Vapor Cooled Shield (VCS) system, utilizing high-conductivity copper and a spiral-shaped ventilation pipe, was integrated to enhance insulation and improve the efficiency of vented hydrogen gas utilization.

A prototype 6m^3 LH2 storage tank was manufactured and validated through performance tests, demonstrating competitive or superior Boil-Off Rate (BOR) compared to leading commercial land-based solutions.

Keywords: Liquefied Hydrogen, Fuel Storage Tank, Novel Design, Hydrogen Powered Ships

Acknowledgement: This research was supported by the grant from National R&D Project "Research Hub Establishment and International Joint Research on Advanced Maritime Mobility (AMM) between Korea and Europe" funded by Ministry of Oceans and Fisheries (RS-2024- 0041020).

---

[a] Presenting Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Design of High-Speed IPMSM Rotor Using CFRP Sleeves

Si-Uk Jung[1,a], Byeong-Hwa Lee[2] and Jae-Woo Jung[1]

[1] Daegu University, E-mail: jsu9085@daegu.ac.kr, jjw@daegu.ac.kr

[2] Korea Automotive Technology Institute, E-mail: bhlee2@katech.re.kr

Speeding up electric vehicle (EV) traction motors is crucial for enhancing power density and energy efficiency, thereby improving vehicle performance. Currently, interior permanent magnet synchronous motors (IPMSM) are widely used, but the risk of permanent magnet separation due to centrifugal force at high speeds requires mechanical reinforcement. These structural constraints may degrade electromagnetic performance. To address this, a Carbon Fiber Reinforced Plastic (CFRP) sleeve design was proposed [1]. CFRP sleeve motors enhance electromagnetic performance by reducing leakage flux and iron loss while maintaining high mechanical rigidity. To fully leverage these advantages, it is important to clearly identify and optimize design factors in trade-off relationships in the CFRP sleeve rotor design [2].

This study proposes a high-speed design and optimization approach by applying a CFRP sleeve to the rotor of the IPMSM Proto model [1], which is currently in mass production for EV traction motors. The design specifications aim to achieve a maximum speed of 25,000 rpm, a maximum torque of 355 Nm, and a maximum output of 150 kW, which are higher than those of the Proto model. In the initial design stage, the Phi-L map was used to set the target range of inductance and flux linkage that met the required specifications, and to design a core shape that could secure rotor rigidity at maximum speed. The safety factor was examined through finite element analysis, and the Incremental Method [3] was utilized to precisely reflect the change in load conditions, thereby calculating reliable

inductance and flux linkage even in the area of low current phase angle. Based on this, the characteristics according to the application of CFRP sleeve were compared and analyzed to derive the advantages and disadvantages of each design. In the detailed design stage, based on the characteristic analysis results, design elements to improve torque and reduce Von Mises stress were reviewed and applied in the initial design model of the CFRP sleeve motor. In this process, in order to shorten the optimization time, a dimensional range for the position and size of the permanent magnets that can satisfy a safety factor of 1.2 was selected. Finally, the optimal design of the CFRP sleeve rotor was performed using a genetic algorithm, considering both mechanical and electromagnetic characteristics. Additionally, a cross-laminated structure was applied to enhance the structural stability of the segmented core and improve manufacturability [4].

The performance analysis of the optimal model based on the d-q axis equivalent circuit

[5] confirmed that it satisfies the target specifications and safety factor while improving average efficiency compared to the Proto model. Additionally, the starting point of the maximum torque per ampere control region was lowered, enhancing control efficiency in the high-speed operating range [6]. Furthermore, the reduction in axial length and permanent magnet usage led to an improvement in power density. The full paper will provide a detailed description of the optimization process and verify the design effectiveness through the fabrication and testing of an experimental model.

---

[a] Presenting Author

Keywords: Carbon fiber reinforced plastic, High speed, Interior permanent magnet synchronous motor, Finite element analysis, Safety factor

References:

[1] S. -U. Jung, D. -S. Kim, J. -S. Lee and J. -W. Jung. 2024. Study on Performance Changes of EV Traction Motor Applying CFRP Sleeve To IPMSM. in IEEE Transactions on Magnetics. doi: 10.1109/TMAG.2024.3509873.

[2] J. -W. Jung, B. -H. Lee, D. -J. Kim, J. -P. Hong, J. -Y. Kim, S. -M. Jeon and D. -H. Song. 2012. Mechanical Stress Reduction of Rotor Core of Interior Permanent Magnet Synchronous Motor. in IEEE Transactions on Magnetics. vol. 48, no. 2, pp. 911-914.

[3] D. -S. Kim, B. -H. Lee, M. -S. Lim and J. -W. Jung. 2024. Calculation Method of d-Axis Inductance Considering Magnetic Saturation and Cross Coupling Effects Under Load Conditions. IEEE 21st Biennial Conference on Electromagnetic Field Computation. pp. 1-2.

[4] J. -W. Jung, K. -T. Jung, B. -H. Lee and J. -P. Hong. 2019. Design and Analysis of Ferrite Magnet Flux Concentrated PMSM With Cross-Laminated Rotor Core Using Equivalent 2-D FEA. in IEEE Transactions on Energy Conversion. vol. 34, no. 3, pp. 1623-1631.

[5] B. -H. Lee, S. -O. Kwon, T. Sun, J. -P. Hong, G. -H. Lee and J. Hur. 2011. Modeling of Core Loss Resistance for d-q Equivalent Circuit Analysis of IPMSM considering Harmonic Linkage Flux. IEEE Transactions on Magnetics. vol. 47, no. 5, pp. 1066-1069.

[6] S. Kim, Y. -D. Yoon, S. -K. Sul and K. Ide. 2013. Maximum Torque per Ampere (MTPA) Control of an IPM Machine Based on Signal Injection Considering Inductance Saturation. in IEEE Transactions on Power Electronics. vol. 28, no. 1, pp. 488-497.

Acknowledgment: This research is a result of the support from Daegu Metropolitan City 2023 Future Mobility Leading Technology Development Project (Project Number: DG-2023-06)

Statistically compatible hyper-reduction for variationally consistent homogenization and its application to diffusion

Jan Hauck[1], **Stephan Wulfinghoff**[1]

[1] Kiel University, Institute for Materials Science, Kaiserstr. 2, 24114 Kiel, Germany,

{jd,swu}@tf.uni-kiel.de

Abstract: We present a statistically compatible hyper-reduction method and its application to time depen- dent diffusion processes in a homogenized two-phase materials consisting of inclusions in a matrix. We use a variationally consistent homogenization [1]. The hyper-reduction method introduces generalized integration points which ensure the consistency with the first and second statistical moment of the fully integrated model [2]. Because diffusion in the matrix is assumed to be much faster than diffusion inside the inclusions, the micro-scale cannot be assumed to be at equilibrium which introduces a time dependence.

Keywords:

* Presenting author

References

[1] Larsson, F.; Variationally consistent computational homogenization of transient heat flow *Int. J. Numer. Meth. Engng* (2010) **81**:1659-1686.

[2] Wulfinghoff, S.; Statistically compatible hyper-reduction for computational homogenization *Computer Methods in Applied Mechanics and Engineering* (2024) **420**:116744.

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

Design of Liquefied Hydrogen Tank Support Structure Considering Structural and Thermal Performance Utilizing Topology Optimization Concept

Ha-yeong Kim [1,a], Gun Woo Kim [1], and Hyun-seok Kim [1,b]

[1] Korea Research Institute of Ships and Ocean Engineering, Alternative Fuels and Propulsion System Research Center, Daejeon, Republic of Korea

Corresponding Author E-mail: hskim85@kriso.re.kr

Ships play a vital role in global trade but also contribute significantly to emissions. To mitigate these environmental concerns, the International Maritime Organization (IMO) has emphasized the importance of adopting eco-friendly alternative fuels. Among these, hydrogen has emerged as a promising option due to its high energy density relative to its mass. However, due to its low volumetric energy density, it requires advanced storage solutions, particularly for vessels with limited space. Storing hydrogen in a liquefied state at -253°C has become a widely adopted approach, but requiring high-performance insulation technologies to ensure efficient and safe storage.

The core of insulation technologies for maintaining cryogenic environments lies in minimizing thermal conductivity. In particular, the support structure between the inner and outer tanks of liquefied hydrogen storage systems plays a crucial role, as its design significantly impacts the overall thermal performance. Reducing the cross-sectional area of these support structures and increasing the distance over which heat is conducted can effectively suppress thermal transfer. However,

such approach may risk the integrity of the structure since the cross- sectional area is usually reduced to minimize the thermal conductivity. Therefore, a balanced approach that considers both thermal conductivity reduction and structural stiffness is essential.

In this study, a topology optimization method is applied to the design of inner-outer tank connecting support structure to achieve an optimal shape that satisfies both structural and thermal performance. Finite element analysis (FEA) is carried out for the initial model to evaluate structural response under mechanical and thermal loads and to identify high level of stress areas, providing foundational data for design improvements. An optimized support structure, obtained from topology optimization results, is found that can minimize the cross- sectional area, enhance insulation performance, and ensure structural integrity under various loading conditions of a target ship compared to the initial model.

Keywords: Liquefied Hydrogen, Liquefied Hydrogen Storage Tank for Ships, Finite Element Analysis, Topology Optimization, Inner-Outer Tank Connecting Support Structure

Acknowledgement: This research was supported by the grant from National R&D Project "Research Hub Establishment and International Joint Research on Advanced Maritime Mobility (AMM) between Korea and Europe" funded by Ministry of Oceans and Fisheries (RS- 2024-0041020).

[a] Presenting Author

[b] Corresponding Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Fourth-order phase field modelling of crack initiation and propagation under combined thermo-mechanical loadings with strong form meshless method

Izaz Ali [1,a], Boštjan Mavrič[1], Božidar Šarler[1,2]

[1] Faculty of Mechanical Engineering, University of Ljubljana, Slovenia, E-mail: izaz.ali@fs.uni-lj.si, bostjan.mavric@fs.uni-lj.si

[2] Institute of Metals and Technology, Ljubljana, Slovenia E-mail: bozidar.sarler@fs.uni-lj.si

This study presents a novel approach for simulating the thermo-mechanical crack initiation and propagation using the fourth-order phase-field method (PFM) with the strong- form meshless local radial basis function collocation method (LRBFCM). The third-order polyharmonic splines, augmented with second-order polynomial augmentation, are used as an interpolation function with LRBFCM to discretise the governing equations of the PF, thermal and mechanical models and solve them staggered. The spectral split method is used for the decomposition of the strain tensor to ensure physically correct crack propagation. The quenching test case is used as a benchmark for validation of the proposed method, where the results were compared with the finite element method (FEM) and experimental results with good agreement. The results of the LRBFCM are obtained using both regular and scattered node arrangements, demonstrating the robustness and ability of the method to accurately predict crack propagation under complex conditions involving steep thermal gradients and extensive mechanical loading. The work represents a first crack propagation simulation under thermomechanical loading using a strong-form meshless method.

Keywords: Fourth-order Phase Field, Meshless Method, PHS, Thermo-mechanics, Quenching

[a] Presenting Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Continuous Unsteady Adjoint Variational Multiscale Method for airfoils applications

Carlo Brunelli [1,*], Bart Janssens[2]

[1]Royal Military Academy, E-mail: carlo.brunelli@mil.be

Abstract: Airfoil optimization using the adjoint-based method has been widely used thanks to its efficiency in computing sensitivities. In this research, the finite element method based on the Variational MultiScale (VMS) method is used to solve the flow and adjoint equations. The derivation of the VMS terms for the resolution of the continuous adjoint problem is shown. The method has been implemented for airfoil design with the aim of improving time-averaged aerodynamic performance. In the implementation Class Shape Transformation (CST) is used to parameterize the control surface to ensure that the obtained geometries are always airfoil-like. In the test case, from a NACA0012 at Re = 1000, AoA = 2.5, a C_L = 0.35 is targeted and achieved. The effect of the time window for time averaging has been investigated, which shows a crucial role for the convergence of the algorithm.

Keywords: Variational MultiScale Method, Adjoint, Airfoils, Optimization

* Presenting author

The exploitation of the adjoint method is a well-established and efficient methodology for evaluating the sensitivities for CFD applications. Airfoil optimization, for different applications, using the adjoint method has been used for more than three decades, [4, 5, 2, 3, 9, 8, 7]. In this study, the Variational MutltiScale Method (VMS), originally introduced by [1], is used to solve the flow and the adjoint set of equations. The FEM formulation based on the VMS stabilization, uses the same order interpolation for velocity and pressure.

The equations governing the adjoint variables are.

R $= - \underline{\phi \mathbf{u}} - \nabla(\phi) - \nabla(\phi)' \cdot \mathbf{u} - \nabla(\phi) \cdot \mathbf{u} - \nu\Delta(\phi)$

madj $\partial t \quad p \quad \mathbf{u} \quad \mathbf{u} \quad \mathbf{u}$

,

$R_{cadj} = -\nabla \cdot (\phi_{\mathbf{u}})$

To obtain the finite element formulation the following dual or adjoint test functions are introduced $\mathbf{v}_\dagger \in V_\dagger$ and $q_\dagger \in Q_\dagger$: $V_\dagger = \{\mathbf{v}_\dagger : \Omega \rightarrow \mathrm{R}^D : \mathbf{v}_\dagger$ is continuous over $\Omega\}$, $Q_\dagger = \{q_\dagger : \Omega \rightarrow \mathrm{R}$: $q_\dagger$ is continuous over $\Omega\}$, where Ω is the fluid domain and D is the dimension (2 or 3) ,and the subscript † denotes an adjoint variable or space. V, $V_\dagger$ and $Q, Q_\dagger$ have respectively the same order and the only differences are at the domain's boundaries. The adjoint galerkin equation becomes:

$$B = \int \nu \cdot \nabla(\mathbf{v}) \odot \nabla(\phi) - q(\nabla \cdot \phi) \, d\Omega + \int \mathbf{v} \odot \underline{\phi \mathbf{u}} - \nabla(\phi) - \nabla(\phi)' \cdot \mathbf{u} - \nabla(\phi) \cdot \mathbf{u} \, d\Omega \quad (1)$$

$G_\dagger \quad \dagger \quad \mathbf{u} \quad \dagger \quad \mathbf{u} \quad \dagger \quad \partial t \quad p \quad \mathbf{u} \quad \mathbf{u}$

And the SUPG and VMS adjoint stabilization terms:

$$B_{SUP\ G}{}^{\dagger} = \int \left(-\mathbf{v}_{\dagger}' \cdot \mathbf{u} - \mathbf{v}_{\dagger} \cdot \mathbf{u} - \nabla(q_{\dagger})\right) \odot \tau_m \mathbf{R}_{\mathbf{madj}}\, d\Omega - \int \tau_c \cdot (\nabla \cdot v_{\dagger}) \odot R_{cadj}\, d\Omega \qquad (2)$$

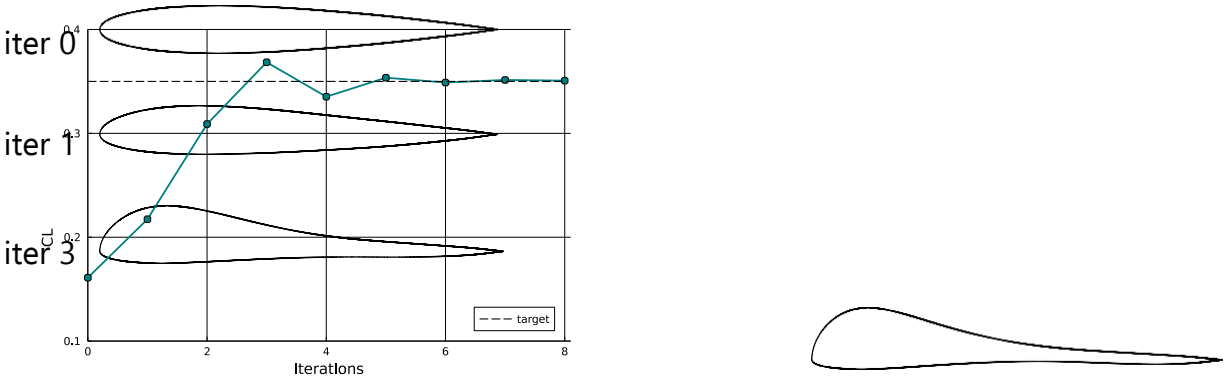


Figure 1: Inverse design of airfoil for C_L^* = 0.35 at *Reynolds* = 1000 and 2.5°: iterationhistory of the time-averaged lift coefficient with a few intermediate shapes

$$B_{VMS} = \int_t \int_\Omega (-\mathbf{u} \cdot (\mathbf{v}_t') \odot \tau_m \mathbf{R}_{\mathbf{madj}} + \nabla(v_t)(\tau_m \mathbf{R}_{\mathbf{madj}} \times \tau_m \mathbf{R}_{\mathbf{madj}}) \, d\Omega \qquad (3)$$

The solution of the adjoint problem requires the complete resolution and storage of the primal flow variables. The optimization algorithm employed in this study is the L-BFGS procedure (limited memory-Broyden-Fletcher-Goldfarb-Shanno) [6]. This method is a limited-memory quasi-Newton approach designed to address nonlinear optimization challenges governed by upper and lower bounds on the design variables. The algorithm is suitable for scenarios where computing information about the second derivative (the Hessian) is challenging.

The methodology has been tested in finding an airfoil with a time-averaged C_L^* = 0.35 for a Reynolds number 1000 and angle of attack 2.5°. A NACA0012 airfoil is used as an initial

guess. Figure 1 depicts the intermediate shapes and the evolution of C_L over the iterations cycles.

References

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

[2] Anderson, W.K., Bonhaus, D.L., 1999. Airfoil Design on Unstructured Grids for Turbulent Flows. AIAA Journal 37, 185–191. https://doi.org/10.2514/2.712

[3] Anderson, W.K., Venkatakrishnan, V., 1999. Aerodynamic design optimization on unstructured grids with a continuous adjoint formulation. Computers & Fluids 28, 443–480. https://doi.org/10.1016/S0045-7930(98)00041-3

[4] Angrand, F., 1983. OPtimum design for potential flows. International Journal for Numerical Methods in Fluids 3, 265–282. https://doi.org/10.1002/fld.1650030306

[5] Beux, F., Dervieux, A., 1992. Exact-gradient shape optimization of a 2-D Euler flow. Finite Elements in Analysis and Design 12, 281–302. https://doi.org/10.1016/0168-874X(92)90038-E

[6] Byrd, R.H., Lu, P., Nocedal, J., Zhu, C., 1995. A Limited Memory Algorithm for Bound Constrained Optimization. SIAM Journal on Scientific Computing 16, 1190–1208. https://doi.org/10.1137/0916069

[7] Castro, C., Lozano, C., Palacios, F., Zuazua, E., 2007. Systematic continuous ad- joint approach to viscous aerodynamic design on unstructured grids. AIAA Journal 45, 2125–2139. https://doi.org/10.2514/1.24859

[8] Schramm, M., Stoevesandt, B., Peinke, J., 2018. Optimization of Airfoils Using the Adjoint Approach and the Influence of Adjoint Turbulent Viscosity. Computation 6, 5. https://doi.org/10.3390/computation6010005

[9] Srinath, D.N., Mittal, S., 2010. An adjoint method for shape optimization in unsteady viscous flows. Journal of Computational Physics 229, 1994–2008. https://doi.org/10.1016/j.jcp.2009.11.019

Partitioned Code Coupling for Multi-scale and Multi-physics Problems Through MUI Library

David R. Emerson*, Omar Ahmed Mahfoze, Wendi Liu

Scientific Computing Department, Science and Technology Facilities Council, Daresbury Laboratory, Warrington WA4 4AD, UK;

* Presenting author; e-mail: david.emerson@stfc.ac.uk

The advances in computer architecture and numerical algorithms have allowed scientists and engineers to perform simulations with greater fidelity and increased realism. These advances are not only in terms of the size of the solved problem, but also in the inclusion of multi- physics phenomena. Monolithic approaches to solving multi-physics problems have been successfully used, but they are limited. As the size and complexity of the problem increases, they become infeasible. For instance, the high-fidelity wind farm simulation would be ranging from large-scale (in hundreds of KM scale) simulation of the atmospheric flows to microscale simulation of the flow around the wind turbines.

The partitioned approach, where different numerical methods and software are used, is a viable alternative that offers flexibility and modularity in solving complex problems. This approach allows as well the use of well-established software with minimal development. However, the partitioned approach comes with its own challenges. In particular, it is highly desirable to be able to couple these disparate sets of codes together in an efficient manner that is also capable of running on modern high-performance computing (HPC) platforms. In our work, we have been advancing the development of the Multiscale Universal Interface (MUI) [1, 2], a lightweight library that facilitates the coupling of any computational software through the use of the Message Passing Interface (MPI). MUI is implemented in C++, with

additional wrappers for C, Fortran, and Python. It is a header-only library that can be adopted by existing solvers with minimum implementation. MUI is a self-contained library with no external dependency (except for MPI) allowing portability in any HPC system. MUI can efficiently utilise more than $O(10^5)$ of MPI tasks to transfer 1 billion points (48GB of data), even with the use of a Gaussian spatial interpolation overhead at each point. MUI transcends the role of a data transfer interface by providing an array of user-friendly functions, including spatial and temporal data interpolation, and iterative coupling algorithms such as the Fixed Relaxation and the Aitken's approaches. Recently, the interpolation algorithms of MUI were developed using SYCL, allowing for high-performance computing across various hardware architectures. This amplifies MUI's effectiveness by providing portability across GPUs from leading vendors, ensuring consistent performance regardless of the hardware. MUI's value lies in its highly generalised approach that treats all data as a time-stamped cloud of points. This approach simplifies coupling between grid-based and particle-based solutions, as well as inherently enabling both volumetric and interface coupling approaches.

A number of multi-physics frameworks have been established by using MUI, for example,

[3] used MUI to couple two particle-based solvers, molecular dynamics (MD) and direct simulation Monte Carlo (DSMC) to enable quick complex multi-scale simulations involving micro, meso and macroscopic elements, as found with problems like evaporation. An open-source framework, ParaSiF was built using the finite volume solver OpenFOAM and the finite element solver FEniCS coupled via MUI, [4] for fluid-structure interaction simulations.

Recently, we developed a multi-scale framework combining the Weather Research and Fore- casting model (WRF) [5] and the CFD solver, Xcompact3D [6]. The aim is to perform high-fidelity simulations of wind farms with realistic initial and boundary conditions. WRF is a widely used numerical weather prediction system for both atmospheric research and operational forecasting. It supports both idealised and real-data simulations using real-time input data for real-time weather forecasting. In this work, WRF is utilised to provide

the ini- tial and inlet boundary conditions for the microscale CFD solver, Xcompact3D. This solver uses high-order schemes and has been successfully applied in atmospheric boundary layer wind-farm simulations, as well as other industrial and academic applications. Both WRF and Xcompact3D are open-source and written in Fortran, and hence MUI Fortran Wrapper is utilised. Results demonstrate the accurate simulation of velocity fields and scalability of the computational framework on HPC systems.

By developing and using a highly scalable and portable coupling library such as MUI, we are now able to tackle a wide range of multi-physics problems that involve two or more computational approaches and solvers. During the conference, we will present MUI and its applications.

Keywords: partitioned approach; multi-physics; multi-scale.

References

[1] Y.-H. Tang, S. Kudo, X. Bian, Z. Li, and G. E. Karniadakis, "Multiscale universal inter- face: a concurrent framework for coupling heterogeneous solvers," *Journal of Computational Physics*, vol. 297, pp. 13–31, 2015.

[2] S. L. S. M. L. W. M. O. A. Tang Y.-H., Kudo, "Multiscale universal interface," 2023. https://doi.org/10.5281/zenodo.10054600.

[3] S. Longshaw, R. Pillai, L. Gibelli, D. Emerson, and D. Lockerby, "Coupling molecular dynamics and direct simulation monte carlo using a general and high-performance code coupling library," *Computers & Fluids*, vol. 213, p. 104726, 2020.

[4] W. Liu, S. M. Longshaw, A. Skillen, D. R. Emerson, C. Valente, and F. Gambioli, "A high-performance open-source solution for multiphase fluid-structure interaction," *International Journal of Offshore and Polar Engineering*, vol. 32, no. 01, pp. 24–30, 2022.

[5] W. Skamarock, J. Klemp, J. Dudhia, D. Gill, Z. Liu, J. Berner, W. Wang, J. Powers, M. Duda, D. Barker, *et al.*, "A description of the advanced research wrf model version 4.3; no," *NCAR/TN556+ STR*, 2021.

[6] P. Bartholomew, G. Deskos, R. A. Frantz, F. N. Schuch, E. Lamballais, and S. Laizet, "Xcompact3d: An open-source framework for solving turbulence problems on a cartesian mesh," *SoftwareX*, vol. 12, p. 100550, 2020.

Homogenization of Mechanical Metamaterials with Self-contact Mechanisms for Programmable Stiffness Using Data-driven Constitutive Models

Moritz Frey[1,*], Sebastian Brandstaeter[1], Alexander Popp[1]

[1]Institute for Mathematics and Computer-Based Simulation, University of the Bundeswehr Munich, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany, E-mail: moritz.frey@unibw.de

Abstract: Mechanical metamaterials are engineered materials designed to exhibit extraordinary macro- scopic properties derived from the mechanical behavior of their microstructure, rather than the intrinsic properties of the base materials. These properties are determined by the design of unit cells, fundamental building blocks that define the material's behavior through their topology and interactions. The ability to control these properties is crucial for applications in adaptive structures, impact absorption, and pro- grammable stiffness materials.

This talk explores the design of unit cells incorporating self-contact mechanisms to achieve mechanical metamaterials with programmable, progressive stiffness properties. Using nonlinear finite element models from computational contact mechanics, we demonstrate how variations in the contact topology enable precise control of macroscopic stiffness characteristics. To enable efficient computational modeling of such materials, we propose data-driven constitutive approaches that replace traditional homogenization techniques such as FE^2, which are often prohibitively expensive, particularly in the context of controllable metamaterials or design optimization of structural components.

In this context, we investigate the applicability of data-driven constitutive models, including machine learning-based approaches, for modeling and predicting the mechanical behavior of unit cells in metamaterials with contact interactions. These approaches integrate stress-strain data and microstructural information, providing a promising pathway for efficient, data-driven homogenization techniques. By leveraging self- contact mechanisms in combination with data-driven constitutive models, we aim to facilitate the design of advanced mechanical metamaterials with programmable stiffness tailored to specific engineering tasks.

Keywords: metamaterials, contact mechanics, programmable stiffness, data-driven constitutive models

---

* Presenting author

A 3-scale computational homogenisation strategy for sheet moulded compounds using material network surrogates.

Ujwal Kishore Jinaga1,∗, Ling Wu1, Andreas Kapshammer2, Kepa Zulueta3, Ludovic Noels1 [1]Computational & Multiscale Mechanical of Materials (CM3), University of Li`ege, Belgium,

E-mail:ujwalkishore.jinaga@uliege.be

[2]Institute of Polymer Product Engineering, Johannes Kepler Universit¨at, Linz, Austria

[3]Leartiker Polymer, Markina-Xemein, Spain

Abstract: Sheet Moulding Compounds (SMC) are composite materials used in automotive components owing to their lightweight, versatility, and more economical manufacturing techniques relative to metallic components. SMCs with thermoset matrices in thick-walled composite applications are subjected to tem- perature variations that ought to be accounted for at the design stage. To perform a numerical analysis of thermoset SMCs, a high-fidelity thermomechanical multiscale model is required to adequately represent the distinct constitutive responses of the polymer and the dispersed fibre-polymer bundles. Consequently, adopting a 3-scale model attributed to the meso- and microscale complexities has been the norm [**1**].

In this work, a carbon fibre and vinyl ester SMC is first-order computationally homogenised using a 3-scale strategy, where the microscopic bundle is modelled in 2D as a combination of fibres impregnated by a ther- mosetting polymer, the mesoscale representation consists of the bundles dispersed in the polymer matrix, and the macroscale is the reference experimental sample. The mesoscale Representative Volume Element (RVE) is generated

using Voronoi tessellation for the bundle placement, whose orientation is sampled directly from CT scans of compression molded SMC tensile test specimens. For fast homogenisation, the micro- and meso-scale problems are surrogated by Interaction-based Material Networks (IMNs), based on a thermome- chanical extension of the methodology developed in [**2**]. IMNs have been shown to be thermomechanically consistent by preserving the form of the laws of conservation in their resolution of the finite element problem, achieved by assimilating similar regions or interactions in the microstructure into a network of nodes.

IMNs are capable of linear elastic and non-linear training. The former has been shown to be efficient for non-porous multiphase microstructures in terms of lower computational expenditure compared to Direct Numerical Simulations (DNS), especially for 3D cases [**2**]. In this work, this is extended to linear thermoe- lastic training for the 3-scale strategy and further non-linear training for plasticity-induced non-linearities at the sample level. The computational speed-up obtained in the 3-scale homogenisation due to the IMN surrogates is shown in comparison with full-field simulations.

Keywords: Sheet moulding compound, 3-scale computational homogenisation, Interaction-based material networks

---

* Presenting author

References

[1] J. G¨orthofer, M. Schneider, F. Ospald, A. Hrymak and T. B¨ohlke. 2020. Computational homogeniza- tion of sheet molding compound composites based on high fidelity

representative volume elements. Computational Materials Science. Vol. 174, pp. 109456.

[2] V. D. Nguyen, L. Noels. 2022. Micromechanics-based material networks revisited from the interac- tion viewpoint; robust and efficient implementation for multi-phase composites. European Journal of Mechanics-A/Solids. Vol. 91, pp. 104384.

Acknowledgements: This research has been funded by the Walloon Region under the agreement no. 2010092-CARBOBRAKE in the context of the M-ERA.Net Join Call 2020 funded by the European Union under the Grant Agreement no. 101102316.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Scale-Independent AI Reduced-Order Model with Rollout Training for Long-Term Flow Prediction

Donghu Guo[1]*, Nathalie C. Pinheiro[1], Claire E. Heaney[1,2], Christopher C. Pain[1,2]

[1] Applied Modelling and Computation Group, Department of Earth Science and Engineering, Imperial College London, London, SW7 2AZ, UK.

donghu.guo21@imperial.ac.uk

[2] Imperial-X, White City Campus, Imperial College London, London, W12 7SL, UK.

Abstract: Governed by partial differential equations (PDEs), fluid flow problems are inherently complex, both spatially and temporally. Over the past few decades, Computational Fluid Dynamics (CFD) has been widely employed to simulate these complex physical processes numerically. However, conventional CFD methods are computationally expensive and time consuming, often requiring days or weeks to generate results.

Reduced-order modelling (ROM) is an effective approach to reduce the computational burden by projecting the high-dimensional original data to a low-dimensional latent space, achieved, typically, by using proper orthogonal decomposition (POD) or an autoencoder. A second neural network is trained to learn the dynamics of the system in latent space. Predictions are then mapped back to the original physical space. However, traditional ROMs are tied to the computational domain associated with the original data. If the domain changes, for example, by increasing in size or by internal features changing location, a new

model needs to be trained from scratch, even if solving the same set of governing equations. The generalisation capabilities of such ROMs are therefore limited.

There are a couple of methods that have explored making predictions with ROMs for domains that do change. Hesthaven et al. [1] parametrise both geometry and physical properties developing a ROM based on POD and a multi-layer perceptron. A lid-driven cavity problem is solved over a parallelogram-shaped domain which is defined by three parameters. We wish to devise a method capable of modelling flow past buildings in a neighbourhood, and would require many and complicated parametrisations if we adopted the approach in [1]. Heaney et al. [2] combine a subsampling approach with a domain decomposition framework to obtain a model which can predict for unseen configurations of buildings. The snapshots are local samples taken from the domain, which capture local flow characteristics of flow around buildings. Having trained a convolutional autoencoder to compress the local solution fields, a second neural network is trained to predict how the latent space variables evolve in time. Each subdomain takes information from neighbouring subdomains and adversarial training was used to improve the stability of the predictions. An unseen domain was then decomposed into subdomains and model predictions for individual subdomains are linked through solutions from the neighbouring subdomains, until the global solution converges. This method enabled a ROM to be trained on air flows around one set of buildings and used to predict for other configurations of buildings on a larger domain.

In this work, we extend the idea of [2], although formulate our new method in a very different way. We explore the potential of CNNs that consist of purely convolutional layers to construct a scale-independent ROM. The ROM consists of a convolutional autoencoder (CAE) for compression and reconstruction, and a CNN for prediction in the latent space This gives the model the flexibility to accept and produce inputs and outputs of any size, thus enabling the scale-independent capability. In the CAE, convolutional layers with a kernel size of 2 and a stride of 2 are used for effective downsampling and upsampling. With

three such layers in both the encoder and decoder, the CAE achieves a compression ratio of 64 in 2D. For prediction in the latent space, an explicit time-stepping scheme is employed, where the prediction model takes variables from two time levels (the previous and the current) and outputs the variable for the next time level. Long-term predictions are then generated by calling the model autoregressively. To ensure robust long-term predictions, we employ a training approach called rollout training [3] to train the prediction model. Unlike traditional training, which calculates the loss for the prediction at a single time level, during the training process, the model is called autoregressively to generate predictions across multiple time levels and calculates the loss over these time levels during the training process. This is similar to the above explicit time-stepping for long-term prediction during inference, but with a much smaller number of time steps, randomly sampled from the entire time period. Our methods are demonstrated using a 2D case study of incompressible flow past buildings. After training, our model is capable of making good predictions for both small and large domains, performing well as a flexible and efficient ROM for the problem.

Keywords: data-driven, scale-independent reduced-order modelling, fully convolutional network, rollout

training, incompressible flow

* Presenting author

References

[1] Jan S Hesthaven and Stefano Ubbiali. Non-intrusive reduced order modeling of nonlinear problems using neural networks. *Journal of Computational Physics*, 363:55–78, 2018.

[2] Claire E Heaney, Xiangqi Liu, Hanna Go, Zef Wolffs, Pablo Salinas, Ionel M Navon, and Christopher C Pain. Extending the capabilities of data-driven reduced-order models to make predictions for unseen scenarios: applied to flow around buildings. *Frontiers in Physics*, 10:910381, 2022.

[3] Kiwon Um, Robert Brand, Yun (Raymond) Fei, Philipp Holl, and Nils Thuerey. Solver-in-the-loop: Learning from differentiable physics to interact with iterative pde-solvers. In H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin, editors, *Advances in Neural Information Processing Systems*, volume 33, pages 6111–6122. Curran Associates, Inc., 2020.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Surrogate model for solid-fluid interaction: a scalable neural-network approach

Nathalie C. Pinheiro[1*], Donghu Guo[1], Hannah P. Menke[2], Claire E. Heaney[1,3], Ahmed H. Elsheikh[2], Christopher C. Pain[1,3]

[1] Applied Modelling and Computation Group, Department of Earth Science and Engineering, Imperial College London, London, SW7 2AZ, UK.

n.pinheiro23@imperial.ac.uk

[2] School of Energy, Geoscience, Infrastructure and Society, Heriot-Watt University, Edinburgh, EH14 1AS, UK.

[3] Imperial-X, White City Campus, Imperial College London, London, W12 7SL, UK.

Abstract: Modelling solid-fluid interaction or multiphase flow requires a set of partial differential equations (PDEs) to be solved together to predict the flow behaviour of the system throughout the domain. For instance, in a solid-fluid interaction problem, the numerical solution of the equations should calculate the concentration of the main components, velocities of the fluid flow and the dissolution of the rock. To numer- ically solve the equations that govern this phenomenon, a spatial discretisation is performed. Conventional high-fidelity physical models require a high resolution to obtain reliable results. Consequently, the time and memory consumption to solve conventional methods is huge. Therefore, it has increased the number of research studies on artificial intelligence

(AI) algorithms to build surrogate models capable of performing a simulation similar to the physical one but in a shorter time or using less computational effort.

This work presents the framework of a machine-learning surrogate model for predicting the fluid flow in porous media. Whereas the techniques presented could be expanded to many fluid flow applications, the model was built to solve the fluid's interaction with the rocks in a carbon storage scenario [1]. Compared with other surrogate models research, such as [2], the application analysed is particularly challenging as the dissolution of the rock caused by the fluid means that the solid field is not static and, consequently, it cannot be used as a special feature capable of helping in adjustments of the future prediction.

Furthermore, another challenge for AI algorithms is the complexity caused by the presence of variables with different distributions in the dataset analysed: the velocities, the concentration of carbon dioxide, and the porosity (solid field). This work will compare some ways of dealing with this, such as different scalings.

In this work, the storytelling behind the current framework is explored, providing the comparison of different strategies, such as coupling an autoencoder for compression with another neural network for prediction [3], a subdomain approach [4] and finally the use of samples for training a grid-invariant network that enables inference over larger (unseen) domains. We define grid invariance as the ability of the neural network to be applied to a domain of any size (although the grid spacing must be the same throughout the domain). Therefore, once the neural network layers respect the characteristics presented in this work, the network can be used for inferencing in larger domains.

Additionally, the dataset used for training contains physical simulation results generated with different structures (i.e. different pore structures). As a consequence, the model can

accurately predict the flow in unseen pore structures and is considered geometry-independent. The main results are shown for an autoencoder and some UNet-based models. In the cases considered, structures based on UNets outperformed the autoencoders, with better results obtained using less training time.

In summary, this work proposes a grid-invariant surrogate model for applications involving rock-fluid inter- action and compares different strategies for developing a machine-learning-based surrogate model. Insights and challenges are discussed and results of the best performing model are presented.

Keywords: Surrogate models; Grid invariance; Geometry invariance; Data-driven models; AI-Enhanced Modelling; Convolutional Neural Network; UNet; Solid-fluid interaction.

---

* Presenting author

References

[1] Julien Maes, Cyprien Soulaine, and Hannah P. Menke. Improved volume-of-solid formulations for micro-continuum simulation of mineral dissolution at the pore-scale. *arXiv preprint*, 2204.07019, 2022.

[2] Shuaixian Wang, Haoran Xu, Yaokun Li, Jiwei Chen, and Guang Tan. IE-NeRF: Exploring transient mask inpainting to enhance neural radiance fields in the wild. *Neurocomputing*, 618:129112, 2025.

[3] Claire E. Heaney, Zef Wolffs, Jo´n Atli To´masson, Lyes Kahouadji, Pablo Salinas, Andr´e Nicolle, Ionel M. Navon, Omar K. Matar, Narakorn Srinil, and Christopher C. Pain. An AI-based non-intrusive reduced-order model for extended domains applied to multiphase flow in pipes. *Physics of Fluids*, 34(5):055111, May 2022.

[4] Claire E. Heaney, Xiangqi Liu, Hanna Go, Zef Wolffs, Pablo Salinas, Ionel M. Navon, and Christopher C. Pain. Extending the Capabilities of Data-Driven Reduced-Order Models to Make Predictions for Unseen Scenarios: Applied to Flow Around Buildings. *Frontiers in Physics*, 10:910381, 2022.

Numerical simualtion of pulsatile blood flow in the pulmonary artery under the influence of pulmonary hypertension

Alibek Issakhov[1*], Aidana Sabyrkulova[1], Aizhan Abylkassymova[1]

[1]Kazakh British Technical University, Almaty, Republic of Kazakhstan, e-mail: alibek.issakhov@gmail.com

The pulmonary arteries (PA) play a key role in blood circulation, carrying blood from the right ventricle to the lungs for oxygenation. The main pulmonary artery (MPA), which originates from the heart, divides into two large trunks: the right (RPA) and left (LPA) pulmonary arteries. Diseases of the pulmonary arteries can cause serious harm to health and even lead to death. One such disease is pulmonary arterial hypertension (PAH), which, if not properly treated, can lead to death within three years. PAH is characterized by high blood pressure and increased stiffness and thickness of the vessel walls, which significantly increases the workload of the heart.

This paper presents a numerical simulation of blood flow in a patient-specific pulmonary artery geometry to study the effect of pulmonary hypertension and associated pathologies such as stenosis and aneurysm on hemodynamics. Six models were investigated: healthy artery, artery with pulmonary hypertension, stenosis, aneurysm, pulmonary hypertension with stenosis, and pulmonary hypertension with aneurysm. Pulsatile blood flow was modeled using a physiologically accurate velocity waveform corresponding to normal and hypertensive conditions. The Carreau rheological model was applied to account for the non- Newtonian behavior of blood, with the flow assumed to be laminar and incompressible. The governing Navier-Stokes equations were discretized using the finite volume method. The analysis focused on the evaluation of pressure distributions, velocity profiles, and wall shear stress. The results showed significant differences between normal and pathological conditions, with pulmonary hypertension leading to increased pressure

and wall shear stress, especially in areas of stenosis and bifurcations. Aneurysms caused localized decreases in flow velocity, while stenosis led to increases in velocity and wall shear stress.

Keywords: numerical simulation, hemodynamics, Carreau rheological model, pulmonary artery, hypertension, aneurysm.

CM3P 2025 - Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Tackling challenges in Bayesian model selection with state-of-the-art techniques.

V Mithlesh Kumar[1,*], Sathyamurthy Hegde[1], Anil Yildiz[1], Julia Kowalski[1]

[1] Chair of Methods for Model-based Development in Computational Engineering, RWTH Aachen University, Aachen, Germany

E-mail: kumar@mbd.rwth-aachen.de

Abstract:

The presence of a myriad of competing computational models in a wide range of scientific and engineering applications poses a formidable challenge when selecting the most plausible model for a given set of obser- vations. Quantifying the uncertainty associated with this model selection process is essential to assess the reliability of these computational models.

We present herein a unified Bayesian model selection workflow leveraging Gaussian Process emulation — a machine learning technique used for non-intrusive physics-based machine learning. The workflow starts with model calibration to generate posterior samples of model parameters based on observations given. These are then used to calculate the marginal likelihood, the basis for our model selection. This process faces two computational bottlenecks: significant computational costs involved in numerous model evaluations during calibration and high-dimensional, intractable integrals in the computation of marginal likelihood. To address the former, we integrated Gaussian

process emulators into the workflow using PSimPy, our in-house Python package, for predictive and probabilistic simulations. For the latter, we conducted a comprehensive review of state-of-the-art methods for computing marginal likelihood, emphasizing techniques based on importance sampling. These techniques were systematically analyzed and validated against multiple standard benchmark problems like the Rosenbrock function, leveraging their analytical solutions. We further explored the limits of these methods by extending the analysis to a novel high-dimensional formulation of the Rosenbrock function [1], designed to test their robustness and scalability.

Building on these insights, we identified and integrated a versatile and scalable marginal likelihood estimator

[2] into our Bayesian model selection workflow. This method leverages normalizing flows — a class of gener- ative models — to address the challenges associated with importance sampling-based estimators, specifically solving the problem of optimal proposal design. We demonstrated our workflow on geophysical free sur- face flows, using AvaFrame, an open-source framework for avalanche simulations. Existing Bayesian model selection workflows often rely on marginal likelihood estimators that are prone to computational inefficien- cies and inaccuracies, particularly in high-dimensional settings. By integrating state-of-the-art techniques into practical applications, our study bridges the gap between methodological advancements and real-world Bayesian model selection challenges.

Keywords: Bayesian Model Selection, Normalizing Flows, Importance Sampling, Model evidence, Bayesian evidence, Generative models, Gaussian process emulators.

* Presenting author

References

[1] F. Pagani, M. Wiegand, S. Nadarajah. 2020. An n-dimensional Rosenbrock Distribution for MCMC Testing. arXiv:1903.09556.

[2] A. Polanska, M. A. Price, D. Piras, A. S. Mancini, J. D. McEwen. 2024. Learned harmonic mean estimation of the Bayesian evidence with normalizing flows. arXiv:2405.05969.

Controlling flexural wave propagation on arrays of gyroscopes and beams, with negative refraction and asymmetric modes

K. H. Madine [1,a], D. J. Colquitt[2]

[1] Department of Applied Mathematics, University of Liverpool, Liverpool, E-mail: k.madine@liverpool.ac.uk

[2] Department of Applied Mathematics, University of Liverpool, Liverpool, E-mail: d.colquitt@liverpool.ac.uk

In this presentation we demonstrate methods to control the propagation of elastic waves with periodic arrays of perpendicular gyroscopes on flexural plates. A perpendicular gyroscope is formed of two perpendicular beams—with the base of the vertical beam attached to the plate—and a gyroscope at the free end of the horizontal beam [1]. This design has similarities with the structure of a wind turbine, and for arrays, wind farms. The analytical model is studied alongside finite element simulations, in which boundary conditions (in the form of applied forces and moments) are used to simulate the presence of the spinners.

We investigate the control over the system afforded by altering parameters such as the rate of spin of the gyroscopes, the length of the beams and the orientation of the gyroscope axes. Particular attention is paid to the asymmetric dispersion surfaces of the system which, in combination with the inherent active chirality of gyroscopes, can be exploited to control the propagation of flexural waves on such arrays of gyroscopes to produce highly unusual wave guiding effects. We demonstrate dynamic chiral Chladni patterns in the attached Kirchhoff plates, unidirectional waves at chiral interfaces and the negative refraction of wave modes across interfaces.

Keywords:

Finite element analysis, flexural waves, gyroscopes, negative refraction

[a] Presenting Author

References:

[1] Madine K. H. and Colquitt D. J. 2024. The perpendicular gyroscope: modal analysis of plate, beam and gyroscope multistructures. Phil. Trans. R. Soc. A.38220230358 http://doi.org/10.1098/rsta.2023.0358

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Multi-scale industrial analysis of multilayered bending plates: The 2D+ approach

J. TRICLOT[1], O. LLOBERAS-VALLS[1,2]*, J. OLIVER[1,2]

[1]Escola T`ecnica Superior d'Enginyers de Camins, Canals i Ports de Barcelona (ETSECCPB), Universitat Polit`ecnica de Catalunya, BarcelonaTech (UPC), Spain,

E-mail: julie.triclot@upc.edu, oriol.lloberas@upc.edu, xavier.oliver@upc.edu

[2]CIMNE – Centre Internacional de M`etodes Num`erics en Enginyeria, Spain, E-mail: olloberas@cimne.upc.edu, oliver@cimne.upc.edu

Abstract: Structures with a multi-layered plate morphology, such as composite laminates, are highly valued in aerospace, naval and automotive industry due to their excellent stiffness-to-density ratio. However, their design process is time-consuming, costly, and requires extensive experimental testing to meet the necessary standards for new product adoption. High-fidelity simulations serve as a promising tool to accelerate this process, yet they struggle to balance accuracy and computational efficiency.

The complexity of these materials is particularly evident in the thickness dimension, which is significantly smaller than the in-plane dimensions. As a result, full 3D computations are impractical since they require extremely thin discretizations to avoid pathological behaviours caused by high element aspect ratios.

To address this challenge, this study adopts the 2D+ multiscale approach introduced in [1]. This methodology leverages dimensional reduction at both the macro- and meso-scales, significantly reducing computation time while preserving the heterogeneous properties through the thickness. The approach is based on computational homogenization, employing 2D plate-like structures with degenerated kinematics at the macro-scale and a 1D Representative Volume Element (RVE) through the thickness at the meso-scale. Importantly, this method is non-intrusive and has been implemented in the commercial software Abaqus as a specialized user element.

This contribution assesses the performance of the Abaqus multi-scale user element in bending-dominated scenarios yielding highly accurate results compared to finely meshed 3D simulations. Stress distributions are effectively captured both in-plane and through the thickness, while computational time is drastically reduced—achieving speed-up factors of three orders of magnitude. The 2D+ approach successfully provides 3D-level accuracy at a computational cost comparable to 2D models. This method presents a compelling alternative to existing numerical techniques for analyzing multi-layered bending plates and offers a solid basis for addressing more complex non-linear material behaviour in these materials.

Keywords: Multi-scale analysis, multilayered bending plates, computational homogenization.

---

* Presenting author

References

[1] Wierna, P., Yago, D., Lloberas-Valls, O., Huespe., A. and Oliver, J., On the Efficient and Accurate Non-linear Computational Modeling of Multilayered Bending Plates. State of the Art and a Novel Proposal: The 2D+ Multiscale Approach. Arch Computat Methods Eng 31, 2451–2506 (2024).

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Evolution and Propagation of Pre-existing Crack in the Core of an Earth- Rockfill Dam Due to Reservoir Impoundment

Anulekha Chakraborty[1,a], Sachin Singh Gautam[2], Arindam Dey[3]

[1] IIT Guwahati, E-mail: canulekha@iitg.ac.in

[2] IIT Guwahati, E-mail: ssg@iitg.ac.in

[3] IIT Guwahati, E-mail: arindam.dey@iitg.ac.in

Cracks in the core of earth-rockfill dams can be induced by many factors, such as temperature variations, soil shrinkage or settling of foundations. Following a change in stress state, the generated cracks can propagate through the core of the dam, thereby endangering its safety and long-term performance. An impoundment of an upstream reservoir can lead to a recognizable increase in hydraulic pressure on the inner faces of initially existing cracks, which eventually triggers the propagation of cracks through the core of the dam. This phenomenon is termed as 'Hydraulic fracturing'. Since the failure of Teton dam in 1976, the occurrence of hydraulic fracturing in the soil core of earth-rock fill dams is considered an important geotechnical problem relating to the safety of such dams.

In this work, hydraulic fracturing in the core of an earth-rockfill dam due to impoundment of reservoir is studied within the framework of eXtended Finite Element Method (XFEM), while employing a traction-separation cohesive behavior in Abaqus/Standard. The propagation of a crack, pre-existing at the upstream face of the core, is investigated. In this context, the water wedging action within the crack is also considered by considering tangential and normal flow within and across the crack.

This study successfully elucidates that after the reservoir is impounded, an initial crack present in the core of the dam propagates further only when a leak-off coefficient is considered, which allows to simulate the normal flow of fluid across the crack. This observation re-enacted the hypothesis that pre-existing cracks in the core of zoned dams are able to grow further upon the action of fluid pressure on the crack surfaces. In this regard, a sensitivity study is conducted to arrive at a suitable value of the leak-off coefficient for the dam. It is envisaged that hydraulic fracturing, leading to the further crack propagation, occurs in the adjacent element just beyond the crack tip when the normal stress perpendicular to the crack plane gets transformed from its compressive state to the tensile state. This study shows that an initial crack present on the upstream face of the core above a height of 50 m from the base (specifically for the dam section chosen in the present study) is likely to propagate further due to water wedging action and pressure generated due to the reservoir impoundment. However, it is observed that initial cracks at any other elevation below the ascertained height (from the base of dam) does not induce further crack propagation. This is attributed to the fact that the compressive stresses due to gravity load of the dam material at larger depths are sufficiently higher. In such scenario, the

[a] Presenting Author

water pressure acting on the crack surface might not be enough to lower the effective stresses to a tensile state. Owing to larger depths from the impounding water level, the reservoir water would also take longer time to seep into those depths since they are comparatively far from the dam upstream face. The study successfully highlights that the upper part of the dam core is more prone to severe crack formations and progressive crack propagation to deeper lengths due to reservoir filling.

Keywords: Earth-rock fill dams; Reservoir Impoundment; Hydraulic Fracturing; XFEM; Water wedging action; Crack propagation.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Quantitative Analysis of Granular Explosives through Examination of Compaction Manufacturing Process

Dimitrios Samaras [1,a], Oliver Blackman [1], Maisey Mathew [2], Dr. Soraia Pimenta [1], Prof. Maria Charalambides [1]

[1] Imperial College London

[2] Atomic Weapons Establishment

Granular explosives are extensively used in both military and civilian applications, often serving as secondary explosives in energetic devices. Ensuring the safe handling of these explosives requires an understanding of their response under external stimuli in accident scenarios. This response is primarily governed by the inhomogeneities present in that material, which develop during the manufacturing process through the compaction of explosive powder into the final product. Herein, an attempt is made to characterise the mechanical properties of granular explosives produced by compacting pentaerythritol tetranitrate (PETN) explosive crystals, modelling the powder ensemble as a continuum. To that extent, the Drucker-Prager Cap material model is employed in the commercial Finite Element (FE) software Abaqus to simulate the compaction process. The calibration of the model is performed through a series of experiments on inert energetic crystals of erythritol, identified in the literature to mimic the mechanical properties of PETN (1). These experiments include compaction of the powder in an instrumented die, diametrical compression of the produced tablet, and uniaxial compression of the tablet. Additionally, an inverse analysis was conducted to determine the material parameters with a limited number of experimental results in conjunction with simulated data. The parameters identified from the above procedures are utilized as inputs for our FE analysis. Subsequently, a parametric investigation is conducted to

evaluate the influence of friction between the powder and the tooling on the final product. The overarching objective of our research is to generate quantitative results for the homogenized microstructure of the material and to establish correlations with its sensitivity. Sensitivity, defined as the material's tendency to react under different mechanical stimuli, is addressed by analysing the relative density distribution output from the model. This holistic approach advances our understanding of the relationship between the manufacturing of granular explosives and their sensitivity, thereby unveiling opportunities for optimizing the manufacturing procedure.

Keywords: PETN, FE, Drucker-Prager Cap

[a] Presenting Author, E-mail: d.samaras22@imperial.ac.uk

References:

[1] Burch AC, Wilde ZR, Bahr DF, Yeager JD. A thermal and nanomechanical study of molecular crystals as versatile mocks for pentaerythritol tetranitrate. Crystals (Basel). 2020 Feb 1;10(2).

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

The Principle of Multiscale Virtual Power applied to Cosserat hyperelasticity

Thiesen, Jos´e L. Medeiros[1,*], Janczkowski, Matheus F.[1], Fancello, Eduardo A.[1]

[1] Department of Mechanical Engineering, Federal University of Santa Catarina (UFSC), Florian´opolis, SC, Brazil, E-mail: joselmthiesen@gmail.com

Abstract:

The study of complex phenomena at the smallest scales of materials with hierarchical microstructure has broad applications across various fields. In recent years, multiscale theories based on the concept of a Rep- resentative Volume Element (RVE) have been extended beyond classical continuum mechanics—originally the focus of early studies [1, 2, 3, 4, 5, 6]—to include electro-mechanical interactions [7], hydro-mechanical coupling [8], fluid motion [9], and other multiphysics phenomena. Most of these models rely on a first-order micro-macro transition, which remains a common assumption. However, incorporating higher-order terms enhances the interaction between scales and mitigates limitations such as the requirement for strict scale separation [10]. In elasticity problems, introducing additional kinematic descriptors, such as second-gradient terms, enables the capture of higher-order deformation modes, allowing for the analysis of micro-scale tor- sional and bending effects [11].

In many materials, especially those with complex microstructures, classical continuum theories fail to describe important physical phenomena because they assume that material points possess only translational degrees of freedom. The micropolar theory, originally introduced by Eringen [12], extends classical mechanics by incorporating local rotational degrees of freedom and couple stresses, enabling the modeling of materials with intrinsic size effects, non-symmetric stress tensors, and independent rotational kinematics. These features are crucial in heterogeneous micropolar materials, such as metallic and ceramic foams, trabecular bone, short-fiber reinforced composites, and granular materials, where microstructural rotations significantly influence macroscopic mechanical behavior. However, most existing multiscale approaches assume a classical macro-scale continuum, which may fail to fully capture the effects of microstructural rotations. A micropolar-micropolar multiscale theory, in which both the macro and micro scales exhibit micropolar behavior, provides a more consistent framework for addressing these limitations by allowing rotational interactions to propagate across scales.

This work presents a micropolar multiscale mathematical formulation based on the Multiscale Virtual Work Method, which systematically incorporates microstructural rotations into the macroscopic balance laws. The study focuses on the fundamental theoretical aspects of the formulation and includes selected benchmark problems that illustrate the influence of micropolar effects in multiscale settings. The results highlight the advantages of a consistent micropolar-micropolar transition, particularly in capturing scale-dependent phenomena and improving the predictive capabilities of multiscale models for complex materials.

Keywords: Multiscale, Cosserat Medium, Large deformations, Soft biological tissues

* Presenting author

References

[1] R. Hill. Elastic properties of reinforced solids: some theoretical principles. Journal of the Mechanics and Physics of Solids, 11(5):357-372, 1963.

[2] R. Hill. A self-consistent mechanics of composite materials. Journal of the Mechanics and Physics of Solids, 13(4):213-222, 1965.

[3] R. Hill. The essential structure of constitutive laws for metal composites and polycrystals. Journal of the Mechanics and Physics of Solids, 15(2):79-95, 1967.

[4] J. Mandel. Plasticit´e classique et viscoplasticit´e. Presses de l'Universit´e de Montr´eal, 1972.

[5] C. Miehe. A computational framework for micro-macro transitions based on homogenization, variational principles, and material symmetry. International Journal for Numerical Methods in Engineering, 46(5):689-735, 1999.

[6] M. Hori and S. Nemat-Nasser. Two-scale micro-macro modeling of a granular medium. Mechanics of Materials, 31(10):667-682, 1999.

[7] H. Berger, B. Michel, and A. Ricoeur. Analytical and numerical homogenization approach for piezoelectric fiber composites. International Journal of Solids and Structures, 42(21-22):5692-5716, 2005.

[8] T. Su and R. J. Detwiler. Computational investigation of water flow and solute transport in hydraulic fractures. Water Resources Research, 47(9), 2011.

[9] P. J. Blanco, S. M. Argerich, and R. A. Feijo´o. Homogenization of the Navier-Stokes equations: Derivation of the Darcy-Forchheimer model for the interstitial fluid. International Journal of Engineering Science, 114:1-11, 2017.

[10] M. Ameen, T. Sadowski, and M. K. Nasyrov. Quantitative analysis of scale effect in gra- dient elasticity theory using molecular dynamics simulations. Computational Materials Science, 143:50-58, 2018.

[11] L. P. Lopes, P. J. Blanco, and R. A. Feij´oo. Assessment of second-gradient homogeniza- tion strategies for heterogeneous materials. Computer Methods in Applied Mechanics and Engineering, 395:114968, 2022.

[12]A. C. Eringen. Theory of micropolar elasticity. Journal of Mathematics and Mechanics, 15(6):909-923, 1966.

Multi-scale Analysis and Design of Materials: a Composite Bayesian Optimisation Strategy

R. P. Cardoso Coelho [1,a], F. M. Andrade Pires [2]

[1] Faculty of Engineering, University of Porto, E-mail: ruicoelho@fe.up.pt

[2] Faculty of Engineering, University of Porto, E-mail: fpires@fe.up.pt

The continuous development of materials with enhanced mechanical properties is crucial to meet the growing demands of modern industries. Not only finding solutions tailored to specific applications is essential, but also quicker design processes are required to maintain competitiveness. Advances in high-performance computing and increasingly accurate numerical models have enabled simulation-based material design, offering a cost-effective alternative to experimental testing. Beyond reducing costs, these approaches provide greater flexibility in problem setup, often accelerate development, and can be fully automated for unsupervised execution. However, efficient optimisation techniques, such as Bayesian optimisation, are essential for rapidly and reliably identifying optimal materials.

In this work, we present a composite Bayesian optimisation framework [1, 2] for the analysis and design of structural materials. This technique has been successfully applied to parameter identification problems and direct material design to optimise specific performance objectives. By leveraging the compositional nature of the objective function, our approach significantly reduces the number of required experiments. Compared to state-of-the-art optimisation methods, composite Bayesian optimisation demonstrates superior performance. Additionally, it is well-suited for the optimisation of stochastic objective functions with noisy observations. We also introduce piglot [3], an open-source Python

package for unsupervised optimisation, which implements these algorithms. The framework's capabilities are illustrated through several numerical examples, including the identification of constitutive parameters in a crystallographic-slip model, the design of a beam cross-section, and the stochastic optimisation of a polycrystalline microstructure.

Keywords: Bayesian optimisation, multi-scale modelling, material design

---

[a] Presenting Author

References:

[1] Cardoso Coelho, R. P., Carvalho Alves, A. F., Nogueira Pires, T. M., Andrade Pires, F. M. (2025). A composite Bayesian optimisation framework for material and structural design. Computer Methods in Applied Mechanics and Engineering, 434, 117516. https://doi.org/10.1016/j.cma.2024.117516

[2] Cardoso Coelho, R. P., Carvalho Alves, A. F., Andrade Pires, F. M. (2024). Efficient constitutive parameter identification through optimisation-based techniques: A Comparative analysis and novel composite Bayesian optimisation strategy. Computer Methods in Applied Mechanics and Engineering, 427, 117039. https://doi.org/10.1016/j.cma.2024.117039

[3] Cardoso Coelho, R. P., Carvalho Alves, A. F., Nogueira Pires, T. M., Andrade Pires, F. M. (2024). piglot: An Open-source Package for Derivative-free Optimisation of Numerical Responses. Journal of Open Source Software, 9(99), 6652. https://doi.org/10.21105/joss.06652

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Mean Field Homogenization Based on the Principle of Multi-Scale Virtual Power and Its Dual: Application to Semi-Crystalline Polymers

Jos´e L. P. Vila-Ch˜a[1,*], A. M. Couto Carneiro[1], Bernardo P. Ferreira[2], F. M. Andrade Pires[1]

[1]Faculty of Engineering of the University of Porto, Porto, Portugal

[2]Brown University, Providence, RI, USA

Abstract: Many engineering materials, such as semi-crystalline polymers, possess heterogeneous, hier- archical, and complex morphologies and require accurate predictions of their macroscopic behavior from underlying microscale geometry and mechanisms. Computational homogenization offers a robust framework for addressing this challenge, bridging scales through nested boundary value problems (BVPs) solved at both macroscopic and microscopic levels. de Souza Neto and coworkers[3] established a complete variational formulation for a multi-scale constitutive theory of solids based on computational homogenization. It rests on the rigorous definition of the space of admissible microscopic displacements, coupled with the Principle of Multi-Scale Virtual Power (PMVP), which degenerates into the well-known Hill-Mandel Principle for the standard first-order homogenization formulation, guaranteeing the energetic equivalence of the virtual power between the two scales.

This work focuses on mean-field homogenization techniques, which simplify the interaction between material phases based on the behavior of each phase in an auxiliary single inclusion problem. These methods provide computational efficiency and acceptable macroscopic accuracy[2], and we seek to integrate them into the Principle of Multi-Scale Virtual Power (PMVP) and its dual, the Principle of Multi-Scale Complementary Virtual Power (PMCVP). We focus on a rigorous definition of the minimal spaces of kinematically and stati- cally admissible fluctuation fields, allowing for incompatible displacements and non-equilibrium stresses. We then consider the different models obtained from more stringent restrictions on this minimal space. These formulations result in homogenization rules that differ from standard volume averages and include models coinciding with the $\tilde{\boldsymbol{S}}$- and $\tilde{\boldsymbol{D}}$ -inclusion models proposed by[3] for large-strain semi-crystalline polymer behavior, as well as the Taylor and Sachs models, which coincide with the minimal and most constrained spaces of admissible fluctuation fields. Their computational efficiency and accuracy are confirmed through numer- ical examples, which consider different geometries such as ellipsoids and laminates and elastic, viscoelastic, and viscoplastic constitutive behaviors. A practical example concerning the simulation of large-strain plastic deformation and texture evolution in high-density polyethylene is also presented[3].

Keywords:

---

* Presenting author

References

[1] EA de Souza Neto and RA Feij´oo, "Variational Foundations of Multi-Scale Constitutive Models of Solid: Small and Large Strain Kinematical Formulation," LNCC Research & Development Report 16 (2006).

[2] S. Nemat-Nasser and M. Hori, Micromechanics: Overall Properties of Heterogeneous Materials, North-Holland Series in Applied Mathematics and Mechanics, v. 37 (Amsterdam; New York: North-Holland, 1993).

[3] B.J Lee et al., "Simulation of Large Strain Plastic Deformation and Texture Evolu- tion in High Density Polyethylene," Polymer 34, no. 17 (September 1993): 3555–75, https://doi.org/10.1016/0032-3861(93)90039-D.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Quantitative Assessment of Fracture Risk in Metastatic Vertebrae: An In Silico Approach

Alkaios Lamprakis1a, Nicholas Ovenden2, Simao Laranjeira3

1 UCL Department of Mathematics, London, UK, E-mail: alkaios.lamprakis.22@ucl.ac.uk

2 UCL Department of Mathematics, London, UK, E-mail: n.ovenden@ucl.ac.uk

3 UCL Department of Mechanical Engineering, London, UK, E-mail: s.laranjeira@ucl.ac.uk

Spinal Metastatic Bone Disease (SMBD) weakens vertebrae by disrupting bone metabolism, making bone brittle and prone to fractures that can lead to spinal cord damage and paralysis [1]. Currently, clinicians rely on imaging, qualitative scoring systems, and their experience to diagnose patients and assess fracture risk, which are often not conclusive in terms of clinical needs [2]. To address these issues, this study proposes a computational framework based on Finite Element Methods (FEM), using the open-source Python-based Firedrake solver [3] to simulate fracture risk in patient-specific spinal geometries.

This novel multi-physics, multi-scale framework aims to accurately simulate fracture initiation and propagation by integrating properties in two scales: macroscopic and mesoscopic. At the macroscopic level the behaviour of bone tissue can be modelled using a poroelastic approach, well-suited for vertebrae due to their porous, fluid-filled trabecular structure. Additionally, tumour-induced bone loss and voids weaken the structure and affect fluid flow, making poroelasticity an ideal choice [4]. To simulate this behaviour a poroelastic fluid continuity equation is employed to relate changes in fluid pressure (p) to volumetric deformations of the porous solid (ϵ), as:

$$\alpha \frac{\partial \epsilon}{\partial t} + \frac{\partial}{\partial t}\left(\frac{p}{M}\right) - \nabla \cdot (k \nabla p) = 0, \quad (1)$$

where α is the Biot coefficient, describing how pore pressure contributes to volumetric strain fluid, M is related to the compressibility of the fluid, and k is the permeability which represents how easily fluid flows through the porous matrix. The model was validated by reproducing the solution of a well-known poroelasticity problem demonstrating that our implementation is able to capture the time-dependent response of fluid pressure to loading.

At the mesoscale, a phase-field model captures damage evolution allowing for a representation of crack initiation and propagation [5]. These models, once coupled, should be able to capture the complex interaction between mechanical loads, fluid pressure, and localized damage evolution within the bone. The framework implemented simulates the fracture initiation and propagation as a phase-field variable (φ), which ranges from 0 (undamaged) to 1 (fully damaged). The fracture growth is simulated based on the Euler–Lagrange equation, balancing the critical energy release rate that characterizes the fracture resistance of the material (Gc) and the elastic strain (ε) energy $\psi(\varepsilon)$, as:

$$\frac{G_c}{l}(1\ \varphi - l\ \Delta\varphi) - 2(1 - \varphi)\psi(\varepsilon) = 0, \quad (2)$$

where l controls the width of the diffusive crack zone.

With this model it is possible to simulate crack formation and growth under varying loading, capturing the changes in local mechanical properties and fluid transport, as summarized in Fig.1. The phase-field model will feed localized damage updates into the poroelastic model, ensuring dynamic interaction. To bridge the macroscopic and microscopic scales, the framework will employ multi-scale homogenization: macroscopic stress and fluid pressure fields inform the mesoscale phase-field model, which in turn provides updated effective material properties and damage information. This coupling is crucial for capturing the evolving fracture network in metastatic vertebrae.

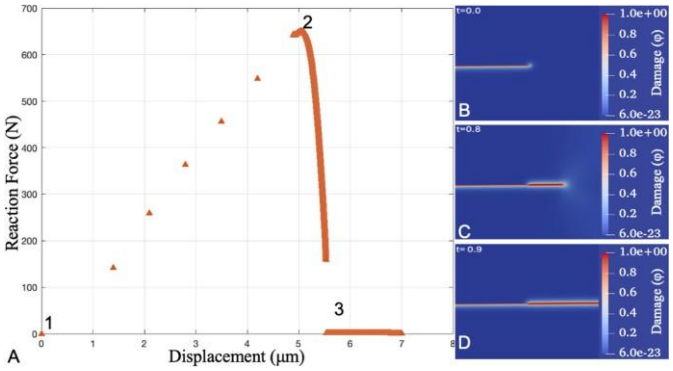


Fig. 1: (A) Force-displacement curve, illustrating material's response under increasing load. The initial elastic deformation (1) is followed by a peak (2), marking crack initiation. The sharp drop indicates fracture propagation as material starts to fail. Finally, the fracture extends through the structure, which can no longer sustain any load, leading to a near-zero reaction force (3). (B, C, D)

crack evolution at different time points, highlighting initiation, propagation, and final fracture.

A key challenge is the numerical non-convergence under complex damage evolution [6]. While preliminary findings show that the separate poroelastic and phase-field models successfully capture fluid-structure interactions and damage evolution, respectively, coupling them is a much more complex task. Even with mesh refinement, the tight coupling between fluid flow and mechanical fields can lead to solver instabilities, requiring specialized stabilization techniques or adaptive meshing to ensure robust simulations [6]. Once these challenges are addressed, the model will be validated against experimental data and applied to clinically

relevant scenarios, with the goal of demonstrating its ability to predict fracture risk under varying loading and disease conditions.

The work presented lays the foundation for the first fully coupled poro-mechanic-phase-field fracture model in Firedrake, providing an open-source computational framework which will be capable of simulating the complex interplay between mechanical loading, fluid transport, and fracture evolution in bone. Integrating these models will enable patient-specific fracture risk assessment and empower clinicians' decision making.

Keywords: Finite Element Methods, Multi-scale, Multi-physics, Multi-uncertainty, Firedrake, Phase-field, Poroelasticity, Metastatic Bone Disease.

---

a Alkaios Lamprakis

References:

1. Okamoto K (2021). Role of RANKL in cancer development and metastasis. J Bone Miner Metab 39:71–81.
2. Murtaza H, Sullivan CW (2019). Classifications in Brief: The Spinal Instability Neoplastic Score. Clin Orthop Relat Res 477:2798–2803.
3. Ham DA et al. (2023). Firedrake User Manual. 1st ed. Imperial College London, University of Oxford, Baylor University, and University of Washington.
4. Scheinpflug J et al. (2018). Journey into Bone Models: A Review. Genes 9:247.

5. Clavijo SP et al. (2022). A coupled phase-field and reactive-transport framework for fracture propagation in poroelastic media. Sci Rep 12:17819.

6. Ambati, M. et al. (2015) A review on phase-field models of brittle fracture and a new fast hybrid formulation. Comput Mech 55

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Effects of Heat Transfer Models on Soot Deposition

Emma Veley[a*], Amy Mensch[a], Ryan Falkenstein-Smith[a], Thomas Cleary[a], Marcos Vanella[a],

Jonathan L. Hodges[b]

[a]National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, USA

[b]Jensen Hughes, 2020 Kraft Drive Suite 3020, Blacksburg, VA

*Corresponding author : emma.veley@nist.gov

Abstract: Fire risk assessments and fire scene reconstructions rely on accurate model predictions of the transport of heat and smoke through a building. These predictions are used to evaluate the consequences to occupants and property resulting from potential fire scenarios. Existing models are well validated in the transport of smoke; however, there is a larger uncertainty in the prediction of the rate at which soot deposits on surfaces exposed to smoke [1]. Soot deposition is a key driver in the damage to artwork [2], sensitive electronics [3], impacts occupant visibility [4], smoke detector activation [5], and is a key indicator in origin and cause analysis in post-fire forensics [6]. Better predictions of soot deposition are needed to improve our ability to quantify the consequences of a fire in the built environment.

Soot deposition is a complex multi-physics phenomenon. It involves buoyantly driven fluid flow resulting from the exothermic combustion reaction, the transport of aerosols within the flow field, mixing with ambient air, and the interactions of the aerosols with the solid surfaces. Thermophoresis, turbulent diffusion, and sedimentation are the three primary mechanisms driving the rate of soot deposition onto a surface. Ther- mophoresis is the occurrence of a force

on the soot particle from the surrounding thermal gradient causing the particle to move in the opposite direction of the thermal gradient. Turbulent diffusion is the process by which smoke particles are transported and impact the surface due to turbulent eddies in the flow and Brownian diffusion. Sedimentation is the process by which gravitational forces acting on the particle drive the soot into a surface. Thermophoretic deposition is typically the largest contributing mechanism to soot deposition [7]. The mass transfer to the surface through thermophoresis depends on the soot concentration near the surface and the fluid temperature gradient at the wall, which can be computed using a convective heat transfer coefficient if the boundary layer is not fully resolved.

The Fire Dynamics Simulator (FDS) is a multi-physics computational fluid dynamics (CFD) software de- veloped and maintained by the U.S. National Institute of Standards and Technology (NIST) [8] which is widely used in the fire protection industry. Researchers have compared the soot deposition predicted by FDS with experiments with varying success. When simulating a laminar flow channel with a controlled thermal gradient, the FDS deposition results were within the uncertainty of the measurements except at the lowest flow rate when buoyancy effects caused reverse flow in the channel [9]. In another study, FDS predicted soot deposited within 2 % on the side walls of a hood apparatus over a burning fuel sample [10]. In a duct study, however, FDS underpredicted the deposition velocity by 45 % [4], which directly relates to an underpredicted deposited amount. Additional experiments are necessary to inform updates to the models used for soot production and deposition [1].

This paper presents data from a series of soot deposition experiments and evaluates the impact of different convective heat transfer models on the amount of soot predicted to deposit onto a surface above a 13.1 kW propene pool fire with a 10 cm diameter. Various configurations were tested, including variations in the distance between the pool fire and the surface, the time of deposition, and the surface material. The three distances between the pool fire and the substrates (97 cm, 128 cm, and 158 cm) were each run for 30 minutes of deposition. The two surface materials – a standard gypsum wallboard (61 cm x 61 cm x 1.3 cm) and a steel sheet

(61 cm x 61 cm x 0.1 cm) – were selected to examine the importance of the thermal properties of the substrate onto which soot is being deposited. The amount of soot was recorded at two radial distances from the center of the board (3.75 cm and 25 cm). The mass loading at these locations was validated against experimental measurements of the same configuration at three times (10 minutes, 20 minutes, and 30 minutes). For comparison between computations and experiments, the gas and surface temperatures were measured with thermocouples installed 2.5 cm below the substrates and on the back side of the substrate respectively.

FDS predictions of soot deposition were generated with three different methods of computing the fluid temperature gradient at the wall. The first two models use the large eddy simulation method where the wall temperature gradient for thermophoretic deposition is computed by assuming a wall heat transfer coefficient. The first method uses the default model for convective heat transfer in FDS which uses the larger of Nusselt correlations for natural convection driven by buoyancy and forced convection parallel to the surface. The second method uses a newly implemented Nusselt correlation for an impinging jet flow [11] rather than the parallel flow correlations. The impingement jet heat transfer model uses an impact velocity which is

calculated based on the stagnation energy per unit mass. The third model for computing the temperature gradient uses Direct Numerical Simulation (DNS) such that the boundary layer adjacent to the wall is resolved by the model. A single configuration is simulated with the DNS model with the gypsum board at 97 cm to evaluate the performance of the two coarser methods and understand how much of the differences between the model predicted and experimentally measured soot deposition is explained by the uncertainty in the convective heat transfer predicted by the models.

Keywords: fire; safety; CFD; smoke

---

* Presenting author

References

[1] T. Beji, J. P. Hidalgo, T. Fateh, J. Floyd, H. Pr´etrel, and A. Hamins, "Compartment fires: Challenges for fire modeling as a tool for a safe design (iafss workshop, april 2021)," *Fire Safety Journal*, vol. 144, p. 104109, 2024.

[2] S. Spafford-Ricci and F. Graham, "The Fire at the Royal Saskatchewan Museum, Part 2: Removal of Soot from Artifacts and Recovery of the Building," *Journal of the American Institute for Conservation*, vol. 39, pp. 37–56, Jan. 2000.

[3] J. S. Newman, G. G. Yee, and P. Su, "Smoke characterization and damage potentials," in *SFPE handbook of fire protection engineering*, pp. 724–744, Springer, 2016.

[4] K. J. Overholt, J. E. Floyd, and O. A. Ezekoye, "Computational modeling and validation of aerosol deposition in ventilation ducts," *Fire technology*, vol. 52, pp. 149–166, 2016.

[5] M. Datta, "Smoke Detector Spacing for High Ceiling Spaces – Phase II," tech. rep., Fire Protection Research Foundation, 2023.

[6] *NFPA 921: guide for fire and explosion investigations*. Quincy (Mass): National Fire Protection Association, 2017 ed ed., 2017. OCLC: 1090344067.

[7] K. M. Butler and G. W. Mulholland, "Generation and transport of smoke components," *Fire Technology*, vol. 40, pp. 149–176, 2004.

[8] K. McGrattan, S. Hostikka, R. McDermott, J. Floyd, C. Weinschenk, and K. Overholt, *Fire Dynamics Simulator, Technical Reference Guide*. National Institute of Standards and Technology, Gaithersburg, Maryland, USA, and VTT Technical Research Centre of Finland, Espoo, Finland, sixth ed., September 2013. Vol. 1: Mathematical Model; Vol. 2: Verification Guide; Vol. 3: Validation Guide; Vol. 4: Software Quality Assurance.

[9] A. E. Mensch and T. G. Cleary, "Measurements and predictions of thermophoretic soot deposition," *International journal of heat and mass transfer*, vol. 143, p. 118444, 2019.

[10] S. Riahi, C. L. Beyler, and J. Hartman, "Wall smoke deposition from a hot smoke layer," *Fire technology*, vol. 49, pp. 395–409, 2013.

[11] J. L. Hodges and R. J. McDermott, "Convective heat transer from impinging flames," in *Proceedings, Fire and Evacuation Modeling Technical Conference (FEMTC)*, 2024.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Modeling and Simulation of Incompatible Deformations in Solids with dislocation microstructure : A Strain-Gradient Approach with Finite Element Implementation

Nicolas Van Goethem[1,*], **Muhammad Adnan Anwar**[2]

[1]Departamento de Matem´atica, Faculdade de Ci^encias, Universidade de Lisboa, Lisboa, Portugal, E-mail: maanwar@fc.ul.pt

[2]Departamento de Matem´atica, Faculdade de Ci^encias, Universidade de Lisboa, Lisboa, Portugal, E-mail: nvgoethem@fc.ul.pt

Abstract: This work deals with the macroscopic modeling of solid continua, typically single crystals, undergoing incompatible deformations due to the presence of microscopic defects like dislocations. We propose a novel approach relying on a geometrical description of the medium by the strain tensor and the representation of internal efforts using zero-th and second-order strain gradients in an infinitesimal framework. The novel kinematic variable is the strain incompatibility, a second-order tensor involving second derivatives of the strain itself. At the same time, energetic arguments allow to monitor the corresponding tangent moduli. We provide mathematical and numerical results to support these ideas in the framework of isotropic constitutive laws. Discretization is made by means of Finite elements. The numerical method is innovative, based on concepts of exterior calculus and the notion of "Complexes", here applied to the so- called elasticity complex. New elements are implemented to address the specific tensor and 4th-order

nature of the equations. We will present the model and a series of numerical simulations on several benchmarks examples in plasticity. Hencky perfect plasticity as well as time-incremental plasticity with hardening will be presented. Comparison with classical models will be provided, in order to assess the validity of our model and highlight its main features. Comparison of the classical and new FE results will be presented as well. This is a joint work with Nicolas Van Goethem (Lisbon), Samuel Amstutz (Avignon), Thien-Nga Lˆe (E´cole polytechnique de Palaiseau) and Francis Aznaran (Notre Dame University).

Keywords: Elasticity, plasticity, strain incompatibility, dislocations, virtual work, dissipation

---

* Presenting author

References

[1] S. Amstutz, N. Van Goethem. 2024. A second-order model of small-strain incompatible elasticity. *Mathematics and Mechanics of Solids*. Vol. 29(3), pp. 503–530. doi: 10.1177/10812865231193427.

[2] D. Arnold. 2018. Finite element exterior calculus. *CBMS-NSF Regional Conference Series in Applied Mathematics*. Vol. 93. doi: 10.1137/1.9781611975543.

[3] F. Aznaran. 2022. Discretisation of Hodge Laplacians in the elasticity complex. PhD Thesis. University of Oxford.

CM3P 2025 - Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems

2–4 July 2025, Porto, Portugal

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Surrogate Modelling for Global Sensitivity Analysis of Biomechanical Arterial Constitutive Models

João Moutinho Gon¸calves[1,*]; Hadi Asgharzadeh Shirazi[2]; Lauranne Maes[3]; Jo˜ao Ferreira[4]; Marco Parente[5]; Nele Famaey[6];

[1]KU Leuven, Leuven, Belgium, E-mail: joaocarlos.moutinhogoncalves@student.kuleuven.be

[2]KU Leuven, Leuven, Belgium, E-mail: hadi.shirazi@kuleuven.be [3]KU Leuven, Leuven, Belgium, E-mail: lauranne.maes@kuleuven.be [4]University of Porto, Porto, Portugal, E-mail: joaof@fe.up.pt [5]University of Porto, Porto, Portugal, E-mail: mparente@fe.up.pt [6]KU Leuven, Leuven, Belgium, E-mail: nele.famaey@kuleuven.be

Abstract: There is growing interest in modelling ascending aortic aneurysms to support decision-making regarding surgical intervention, which stems from the high mortality rates associated with this condition and the inadequacy of current criteria in accurately identifying patients who require surgical intervention [1]. However, arteries are highly complex structures, and computational models struggle to fully capture all their intricacies, such as material behaviour, histological architecture, blood-wall interaction, etc. [2]. Additionally, as more complex models are formulated to depict their real-life behaviour, challenges related to simulation time and resource constraints arise, particularly when many evaluations of the model are needed [3]. A promising solution for these increasing computational costs lies in surrogate models, simplified approximations of high-fidelity models [4]. Thus, this project has the dual objective of advancing the understanding of biomechanical modelling for arteries and integrating data-driven surrogates in a modelling framework.

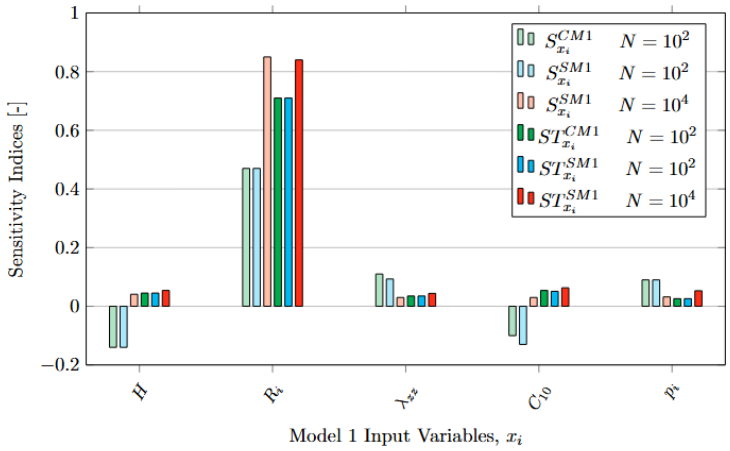
The methodology was structured into six phases: for the first one, three models (CM1, CM2, CM3) were de- veloped to simulate arterial behaviour as an incompressible thick-walled hollow cylinder under loading, each incorporating a different material model (Neo-Hookean, Gasser-Ogden-Holzapfel [5] and the homogenized constrained mixture theory to predict growth and remodelling phenomena[6]). The major distinguishing factor between the models is their complexity, which is represented either in the number of variable fea- tures, the number of material layers being modelled, or computational effort required for execution. In the second phase, to sample inputs for the models (which included material, geometric and loading parame- ters), hypercubic spaces were constructed centred around reference values for each feature variable. Both training/validation and testing datasets were generated, with the testing spaces being designed as broader extensions of the training spaces in order to evaluate model generalization over a wider range of inputs. The third phase consisted of sampling inputs from the hyperspaces using random Latin Hypercube, and recording the computed outputs (r_i, the deformed inner radius). Additionally, output rejection was performed based on physical and computational criteria. In the fourth phase, Gaussian Process Regressions were trained on the generated data with the aid of MATLAB Regression App. This type of architecture proves useful given its stochastic nature. For the fifth phase, in order to assess the predictive accuracy of the surrogates, the surrogate and constitutive outputs were compared for the inputs of the same dataset. For the final phase, Sobol indices were calculated using 100 outputs from the surrogates and 100 outputs from the constitutive models to allow for direct comparison. By leveraging the computational efficiency of the surrogates, indices were also calculated using 10000 samples.

At the end of the project, the developed surrogates proved to accurately predict the deformed inner radius in most cases ($R^2 > 0.8$). However, there was an expected decrease in accuracy as inputs were sampled from broader hyperspaces, which is visible in the flattening of the relative residuals distribution (Figure

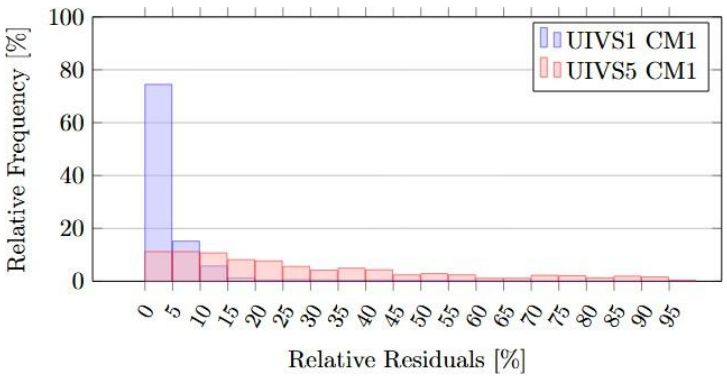
1. (b), where UIVS5 is a broader hyperspace than UIVS1). Regarding the global sensitivity analysis, the undeformed inner radius R_i proved to be the most impactful input feature in the computation of r_i across the different models. Additionally, by using 10000 outputs from the surrogates, more accurate Sobol indices were obtained with greater efficiency compared to calculating the same number of outputs using the constitutive models (Figure 1. (a) shows, for example, that using $N = 100$ resulted in negative 1st-order indices for H and C_{10}, which is theoretically impossible, while using $N = 10000$ with the surrogate allowed for positive indices).

To conclude, when modelling arteries as thick-walled hollow cylinders under loading, the pre-deformation inner radius emerged as the most influential input affecting the deformed inner radius across all mod- els. Moreover, surrogate modelling successfully mitigated the excessive computational costs associated with high-sample number Sobol index calculations, which would be impractical using constitutive models alone. This demonstrates the potential of surrogate models for efficient and accurate evaluations in biomechanical

simulations. However, their effectiveness depends on several factors such as the number of training samples and the breadth of the training space.



(a) Bar chart representing the Sobol indices for CM1



(b) Histogram of relative residuals of UIVS1 CM1 and UIVS5 CM1

Figure 1.: (a) - Each cluster pertains to the indices of a given input variable: for a sample size of $N = 100$, the first-order and total effect indices were computed using constitutive (S^{CM1} and ST^{CM1}) and surrogate (S^{SM1} and ST^{SM1}) outputs; for a sample size of $N = 10000$, only the surrogate outputs were used. The inputs are: undeformed wall thickness H, undeformed inner radius R_i, axial stretch λ_{zz}, material parameter C_{10}, and internal pressure p_i. (b) - The chart represents the relative frequency (number of

occurrences divided by the number of samples) of the relative residuals (the residual divided by the real output). The blue is associated with inputs sampled from hyperspace UIS1 of model 1, and red with inputs sampled from hyperspace UIS5 of model 1 (which is a broader space than UIS1).

Keywords: Arterial Biomechanics, Multi-scale modelling, Constitutive modelling, Surrogate Modelling, Global Sensitivity Analysis

---

* Presenting author

References

[1] Smoljki´c, M., Fehervary, H., Van den Bergh, P., Jorge-Pen˜as, A., Kluyskens, L., Dymarkowski, S., ... & Famaey, N. (2017). Biomechanical characterization of ascending aortic aneurysms. Biomechanics and modeling in mechanobiology, 16, 705-720.

[2] Rajagopal, K. R., & Rajagopal, K. (2020). Modeling of the aorta: complexities and inadequacies. Aorta, 8(04), 091-097.

[3] Bi, S., Beer, M., Cogan, S., & Mottershead, J. (2023). Stochastic model updating with uncertainty quantification: an overview and tutorial. Mechanical Systems and Signal Processing, 204, 110784.

[4] Koziel, S., & Pietrenko-Dabrowska, A. (2022). Fundamentals of data-driven surrogate modeling. In Surrogate Modeling For High-frequency Design: Recent Advances (pp. 1-37).

[5] Gasser, T. C., Ogden, R. W., & Holzapfel, G. A. (2006). Hyperelastic modelling of arterial layers with distributed collagen fibre orientations. Journal of the royal society interface, 3(6), 15-35.

[6] Cyron, C. J., Aydin, R. C., & Humphrey, J. D. (2016). A homogenized constrained mixture (and mechanical analog) model for growth and remodeling of soft tissue. Biomechanics and modeling in mechanobiology, 15, 1389-1403.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Toward a new PGD approach for the numerical simulation of elongated structures

Frédéric Legoll1,∗, Ludovic Chamoin2, Arthur Leb´ee3, Jean Ruel(3)

[1]ENPC and Inria, E-mail: frederic.legoll@enpc.fr

[2]ENS Paris-Saclay, E-mail: ludovic.chamoin@ens-paris-saclay.fr

[3]ENPC, E-mail: {arthur.lebee,jean.ruel}@enpc.fr

Abstract: Elongated structures such as beams, plates or shells, are present in many mechanical systems. Efficiently simulating their behaviour is challenging. Effective models stemming from classical theories (such as the Kirchhoff-Love theory for plates) are justified in the limit of small thickness, and do not necessarily capture the solution for intermediate thickness. On the other hand, direct 3D simulations of the elastic behaviour of such structures may be suboptimal since they do not use the fact that one of the dimension of the system is small.

We will show how to use model order reduction, and in particular the Proper Generalized Decomposition (PGD) method [1], to address such multiscale problems. The PGD method is based on the idea of variable separation, and we use it here to separate the two plane variables from the transverse variable (in the direction of small thickness).

A first approximation consists in looking for the solution of the elasticity problem as a single product of a function of the two plane variables times a function of the tranverse variable, leading to a significant computational cost reduction compared to a full 3D resolution. We will show that this approach however

does not lead to an accurate approximation, and we will explain this flaw on the basis of plate theories. We will then explain how to adapt the PGD approach, in order to obtain accurate approximations. The efficiency of the resulting approach will be illustrated on the basis of several numerical examples.

Keywords: thin structures, reduced order modelling, asymptotic analysis

* Presenting author

References

[1] F. Chinesta, R. Keunings and A. Leygue, The Proper Generalized Decomposition for Advanced Numerical Simulation: A Primer, Springer, 20

Parallel performance of the pseudospectral method applied to the kinematic dynamo problem

Yuan Dongliang1, Constantin Zhukov1, Roman Chertovskih [2,*] [1]Computational Mathematics and Cybernetics faculty, Lomonosov Moscow State University, Russia,

E-mail: ydl747285133@gmail.com, zhukov k@cs.msu.ru -

[2] SYSTEC-ARISE Research Center for Systems and Technologies, Faculty of Engineering, University of Porto, Portugal, E-mail: roman@fe.up.pt

Abstract:

Complex fluid flow phenomena in the presence of electromagnetic fields is the topic of magnetohydrodynam- ics. We study the dynamo problem – generation of a magnetic field by the flow of an electrically conducting fluid. This problem is of interest in geo- and astrophysics (evolution of planetary and stellar magnetic fields), as well as for electromagnetic technological processes (for example, in the cooling processes of nuclear reac- tors using liquid metals). In the cooling processes of nuclear reactors, it is necessary to create a cooling flow stable to magnetic disturbances (i.e. a non-generating flow). The problem in question is important not only for current reactors [1], but also for future fusion reactors, where liquid metals are considered a potential medium for heat transfer [2].

Solving the kinematic dynamo problems is demanding computationally. In the talk we plan to present our recent results of the ongoing study aiming to answer the question: What is the most efficient computational platform to solve the kinematic dynamo problem by the pseudospectral method?

For a given incompressible three-dimensional steady flow **v**(**x**) of an electrically conducting fluid, we consider the kinematic dynamo problem [3]:

$$\frac{\partial \mathbf{b}}{\partial t} = \eta \nabla 2\mathbf{b} + \nabla \times (\mathbf{v} \times \mathbf{b}), \quad (1)$$

for a solenoidal magnetic field **b** = **b**(**x**, *t*). Here η is the magnetic diffusivity, characterizing the electrical properties of the fluid. The flow and magnetic field are assumed to be periodic in all spatial directions with period 2π.

For a given value of the magnetic diffusivity and a flow, numerical solution of (1) is computed using the pseudospectral method [4]. The magnetic field is presented as a Fourier series in all spatial directions, the system of ordinary differential equations for the Fourier coefficients is solved numerically by the standard fourth-order Runge-Kutta method with a constant time step τ . All derivatives in the r.h.s. of (1) are computed in the spectral space, the cross product of the flow and magnetic field is computed in the physical space, forward and backward fast Fourier transforms (FFTs) are used to switch between the spaces. We use FFTs implemented in the libraries FFTW [5] and P3DFFT [6]: the parallel implementation (for distributed memory) of three-dimensional Fourier transformations were used from the P3DFFT, using one-dimensional FFTs from the FFTW. For implementations on GPU the cuFFT library is used.

In computations we used: η = 0.03, spatial resolution of 1024 Fourier harmonics in each direction and t√ime

step $\tau = 10^{-4}$. The flow was chosen to be **v**(**x**) = 2 (sin(x_2) cos(x_3), cos(x_1) sin(x_3), sin(x_1) cos(x_2)) ⁄ 3,

proved to generate magnetic field for η 0.56. To test the codes, we checked that evolution of the magnetic

energy was in agreement with the dominant eigenvalue of the magnetic induction operator (see [7] for details on the kinematic dynamo as an eigenvalue problem).

For numerical experiment we use the following supercomputers. The Oblivion[1] supercomputer (hosted at the University of E´vora, Portugal) consisted of two partitions, old: 58 nodes, each containing 2 Intel Xeon Gold 6154 (18 cores, 3GHz) and 188 GB RAM; and new: 30 nodes, each containing 2 Intel Xeon Gold 6354 CPU (18 cores, 3GHz) and 250 GB RAM. For our experiments we used only nodes from the new partition, because of larger memory size available and higher computational performance (although the clock frequencies and number of cores are the same, both supports Intel AVX-512 instructions, the cashes of the 6354 CPUs are significantly larger). We used optimizing C and C++ compilers from the Intel oneAPI version 2023.2.0 to compile our codes and the FFT libraries mentioned above. Our preliminary results show the following scaling: using one node (32 cores) we obtain speed-up of 15, on two nodes the codes runs 24 times faster than the sequential one, the minimal time is obtained on 16 nodes, with the speed-up of 78 times.

[1]https://catedrahpc.uevora.pt

We have also used the MSU-270 supercomputer (hosted by the Lomonosov Moscow State University, Russia): 32 nodes, each containing 2 AMD EPYC 7742 CPU, 64 core, 2.25 GHz and 8 NVIDIA Ampere A100 GPUs. In contrast to the Intel's compilers on the Oblivion, we used C and C++ provided by GNU. We have obtained the following scaling on CPUs: using one node (128 cores) the speed-up is 17, the minimal time is obtained on 32 nodes, with the speed-up of 170 times. We have found that our codes runs on 8 GPUs about 830 times faster than on one core of the AMD EPYC 7742 CPU.

Currently, we perform measurements of the computational performance of our codes on the Deucalion cluster (hosted by the Minho Advanced Computing Center[2], Portugal). For comparison, we plan to use all three partitions available: ARM (1632 nodes, each with 1 Fujitsu ARM A64FX CPU, 48 cores, 2GHz), x86 (500 nodes, each with 2 AMD EPYC 7742, 64-core, 2.25 GHz) and GPU (33 nodes, each with 4 NVIDIA Ampere A100 GPUs). We plan to study *i*) how slower the codes perform on ARM CPUs using the same amount of computational processes and *ii*) if runs on the GPUs outperform the runs on the CPUs. All these are topics of the ongoing research.

The simulations have been carried out on the Oblivion and Deucalion supercomputers supported by the the Foundation for Science and Technology (FCT, Portugal) in the framework of the calls for computational projects (refs. 2022.15706.CPCA, 2023.10674.CPCA and 2024.07885.CPCA). RC acknowledges the financial support of the FCT in the framework of the Associated Laboratory – Advanced Production and Intelligent Systems (AL ARISE, ref. LA/P/0112/2020) and the R&D Unit SYSTEC (Base UIDB/00147/2020 and Programmatic UIDP/00147/2020 funds).

Keywords: Magnetohydrodynamics; Spectral Methods; Parallel Processing; GPU Computing

* Presenting author

References

[1] Alemany A., Marty P., Plunian F. and Soto J. 2000. Experimental investigation of dynamo effect in the secondary pumps of the fast breeder reactor Superphenix. Journal of Fluid Mechanics, Volume 403, pp. 263-276.

[2] Heinzel A., Hering W., Konys J., Marocco L., Litfin K., Mu¨ller G., Pacio J., Schroer C., Stieglitz R., Stoppel L., Weisenburger A. and Wetzel T. 2017. Liquid metals as efficient high-temperature heat-transport fluids. Energy Technology, Volume 5, pp. 1026-1036.

[3] Moffatt H.K., Dormy E. 2019. Self-Exciting Fluid Dynamos. Cambridge Texts in Applied Mathematics, Cambridge University Press.

[4] Peyret R. 2002. Spectral Methods for Incompressible Viscous Flow. Springer.

[5] Frigo M., Johnson S.G. 2005. The Design and Implementation of FFTW3, Proceedings of the IEEE, 93(2), pp. 216-231.

[6] Pekurovsky D. 2012. P3DFFT: a framework for parallel computations of Fourier transforms in three dimensions, SIAM Journal on Scientific Computing 2012, Vol. 34, No. 4,

pp. C192-C209.

[7] Rasskazov A., Chertovskih, R., Zheligovsky V. 2018. Magnetic field generation by point- wise zero-helicity three-dimensional steady flow of an incompressible electrically con- ducting fluid. Physical Review E, 97(4), 043201.

[2] https://www.macc.fccn.pt

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

An Iterative Method for Elastic Multiple Scattering Coupled with a High Order Local Farfield Expansion ABC

Vianey Villamizar[1,*], **Jordan Shepard**[2]

[1,]Brigham Young University, E-mail: vianey@math.byu.edu

[2,]Brigham Young University, E-mail: jsheppard@mathematics.byu.edu

Abstract: We have developed a highly accurate and high order numerical method for elastic multiple scattering by coupling an iterative numerical method with local high order absorbing boundary conditions (ABC) based on Karp's farfield expansions.

Keywords: Absorbing boundary conditions, Iterative method, Elastic multiple scattering

* Presenting author

1 Formulation of the elastic multiple scattering problem and construction of its high order local absorbing boundary condition (ABC)

We focus our study on finding the displacement wave, u, obtained from the scattering of a time-harmonic plane elastic wave, $\mathbf{u}_{inc}(\mathbf{x})$ from M multiple obstacles embedded in an elastic medium in two dimensions. This medium is homogeneous, isotropic, and linear with constant physical properties, density ρ, and Lame constants μ, λ. The boundary of the m-th obstacle is denoted by Γ_m and we denote the unbounded region in the exterior of Γ_m by Ω_m, for

m = 1, . . . M. Hence, the common scattered region is $\Omega = \bigcap_{m=1}^{M} \Omega_m$ and the boundary of the

full problem is $\Gamma = \bigcup_{m=1}^{M} \Gamma_m$, where M is the total number of obstacles. We showed in our

previous work [1] that this scattering problem can be modeled by two elastic potentials φ_{sc}

and ψ_{sc} satisfying the following BVP for the Helmholtz equations,

$$\Delta\varphi_{sc} + k^2\varphi_{sc} = 0, \quad \Delta\psi_{sc} + k^2\psi_{sc} = 0, \quad \text{in} \quad \Omega, \quad (1)$$

p s

Soft Scaterrer boundary condition: $\mathbf{u} = -\mathbf{u}_{inc}$, on Γ (2)

or hard scaterrer boundary condition: $\sigma(\mathbf{u}) = -\sigma(\mathbf{u}_{inc})$ on Γ, (3) $\lim r^{1/2} (\partial_r\varphi_{sc} - ik_p\varphi_{sc}) = 0$, $\lim r^{1/2} (\partial_r\psi_{sc} - ik_s\psi_{sc}) = 0$. (4)

$r\to\infty$ $r\to\infty$

where **u** and σ represent the displacement vector and the stress tensor, respectively. They are represented in terms of the scalar potentials φ_{sc} and ψ_{sc} by well-known formulas. We

solve this problem by transforming it into a system of M single scattering problems and imposing the following Karp's farfield expansions high order local absorbing boundary conditions (KFE- ABC) defined in [3] on a circular artificial boundary C_m for each obstacle,

$$\varphi^{\infty,p}(r,\theta) = H(k_p r) \times F_{m,l}(\theta_m) + H(k_p r) \times G_{m,l}(\theta_m) =: K^p(r,\theta), \quad (5)$$

$$\psi^{\infty,s}(r,\theta) = H(k_s r) \times F_{m,l}(\theta_m) + H(k_s r) \times G_{m,l}(\theta_m) =: K^s(r,\theta). \quad (6)$$

A detailed description of this transformation is found in our previous work [2]. A brief description is as follows:

1. We decompose the scattered displacement wave **u** into the sum of M single scattered

displacements corresponding to each scatterer. It means **u** = LM $_{m=1}$**u**$_m$, It is also known that the wave emitted from the boundary Γ_m of a given obstacle, is determined by the incident wave and the waves emitted from the boundaries Γ_{m^-} of all other scatterers.

Reciprocally, the wave emitted at the boundaries of each one of the other scatterers is in turn influenced by the wave emitted by the given scatterer. For the displacement

u$_m$, this means that **u**$_m$ = in M **u** , on Γ_m, for m = 1 . . . M.

−**u** c $_{m^-=1}$ m

m^-

6=m

2. We introduce circular artificial boundaries C_m (m = 1 . . . M) to enclose each individual scatterer. These artificial boundaries C_m divide each infinite domain Ω_m in a bounded one, $\overset{m}{\Omega^-}$ (enclosed between the obstacle boundary Γ_m and the circular artificial C_m) and the unbounded region $\Omega^+ = R^2 - \Omega^-$.

m m

3. We place a KFE-ABC in terms of the scalar potentials for each artificial boundary C_m. As a result, each of the unbounded single scattering problems for the potentials φ_m and ψ_m are transformed into bounded ones.

4. Imitating the procedure at [2] for the acoustic case, we decouple the scatterer bound- ary condition at each Γ_m by rewriting it in iterative form. We adopt Gauss-Seidel- and Jacobi-type iterative formulations. As a result, the original scattering problem is reduced to a sysstem of M uncoupled single scattering problems.

5. Finally, we use finite differences method to approximate the solution for each one of these problems at every iteration step. The iteration process stops when the difference

between the scattered waves $\mathbf{u}^{(n)}$ and $\mathbf{u}^{(n-1)}$ in Ω_m is less than a specified tolerance, tol, for all m = 1 . . . M.

We have performed numerical experiments that show high accuracy and high order of con- vergence. We will discuss them during our presentation at the conference.

References

[1] D. Grundvig, High order numerical methods for problems in wave scattering, Master's thesis, Brigham Young University (2020).

[2] V. Villamizar, T. Khajah, J. H. Hale, Highly efficient iterative method for multiple scattering with high order local ABC, Comput. Methods Appl. Mech. Engrg. 430 (2024) 28.

[3] V. Villamizar, S. Acosta, B. Dastrup, High order local absorbing boundary conditions for acoustic waves in terms of farfield expansions, Journal of Computational Physics 333 (2017) 331–351.

Predicting the Macro Compression Strength of Masonry via Probabilistic Discontiuum-Based Analysis

Rhea Wilson[1] and Bora Pulatsu [2,a]

[1] Carleton University, E-mail: rheawilson@cmail.carleton.ca

[2] Carleton University, E-mail: bora.pulatsu@carleton.ca

Simulating the fracture mechanism and strength of masonry composite subjected to compression loading is a challenging task when considering the significant uncertainty in the material properties and existing meso- or macro-scale damages in the masonry constituents (brick and mortar). As a composite material, the mechanics of masonry is influenced by the strength of its constituents and the quality of the bond between them. Numerous factors can affect the overall load-carrying capacity and damage progression in masonry composite, including low workmanship quality, strength and stiffness incompatibility between materials, environmental factors, and mechanical wear. The present study aims to better understand the damage progression in masonry prisms, including the material uncertainty and macroscopic damages at the brick and/or mortar. To achieve this goal, a discontinuum-based computational model is proposed where brick, mortar, and brick-mortar interfaces (bond) are explicitly represented in the simulation [1]. Specifically, the masonry specimens are represented as mechanically interacting discrete rigid triangular blocks, allowing cracks to propagate through the material using the discrete element method (DEM). Damage progression under compression loading is tracked and visualized, providing insight into crack formation, propagation, and fracture. Once the adopted computational modeling approach is validated, the micro-strength and stiffness properties of the masonry constituents are systematically varied, considering their spatial variation to explore the influence of material uncertainty

on the macro compression strength. Furthermore, non-cohesive joint planes are defined at the units using a newly developed crack inclusion algorithm to replicate the mechanical damage in the material and investigate its effect on the overall composite system. The proposed probabilistic analysis approach offers interesting insights into the complex fracture mechanism in masonry. It also provides valuable outcomes regarding the significant influence of micro-scale parameters on the macro strength and behavior of masonry composite.

Keywords: Computational Modelling, Fracture Simulations, DEM, Material Uncertainty

[a] Presenting Author

References:

[1] . Pulatsu, B., 2023. Coupled elasto-softening contact models in DEM to predict the in- plane response of masonry walls. Computational Particle Mechanics, 10(6), pp.1759-1770.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

A discrete dual finite volume method for the convection-diffusion equation: toward cold-plasma modeling.

Thomas Bonnafont[1,*], Delphine Bessi`eres[2], Jean Paillol[2]

[1]Lab-STICC, ENSTA, Institut Polytechnique de Paris, Brest, France E-mail: thomas.bonnafont@ensta.fr

[2]Universit´e de Pau et des Pays de l'Adour, E2S UPPA, SIAME, E-mail: firstname.surname@univ-pau.fr

Abstract: To model cold plasma one needs to solve a system of convection-diffusion and Poisson equations as [3]. In [1], we proposed a discrete dual finite volume (DDFV) method to solve the Poisson equation with non-homogeneous jump conditions. This work is thus devoted to solving the convection-diffusion equation, in the framework of [2], using a self-consistent DDFV scheme to then apply it to cold-plasma modeling. Contrary to [2], mixed boundary conditions, and both the steady-state and time varying equations are studied. Numerical tests are proposed to show the convergence rate of the method in different configurations.

Keywords: convection-diffusion equation, finite-volume, DDFV, diamond scheme

* Presenting author

In this work, we focus on the modeling of cold plasma, which requires solving the following system of equations [3]:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) - D\nabla \cdot (\nabla n) - \alpha_{\text{eff}} n|\mathbf{v}| = 0$$

$$\nabla \cdot (\nabla V) = f, \qquad (1)$$

where $\mathbf{v} = \mu\mathbf{E}$, $\mathbf{E} = -\nabla V$, and D and α are given constants. Since the velocity field $\mathbf{v}$ is derived from the potential V, achieving high accuracy in solving the Poisson equation is crucial. In [1], a Discrete Duality Finite Volume (DDFV) scheme was proposed to solve this equation with high accuracy, even on distorted meshes.

Here, we extend this approach by focusing on the first equation. Specifically, we aim to develop a self-consistent DDFV scheme for the convection-diffusion equation:

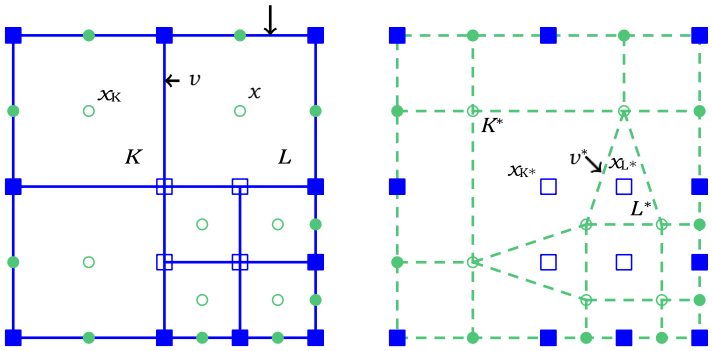
$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) - D\nabla \cdot (\nabla n) - \gamma n = \bar{f}, \qquad (2)$$

where f is a source term, $\mathbf{v}$ is a given vector field, and γ is a constant. We also consider mixed boundary conditions. Our scheme relies on the DDFV direct discretization for the diffusion operator, as in the Poisson case, while the convection term is approximated using a finite volume approach based on the primal/dual mesh of DDFV. Figure 1 illustrates an example of this mesh structure, which is key to our discretization strategy. By leveraging

the dual mesh and an affine interpolation of the field values on each edge, we construct a self-consistent approximation of the gradient.

We first validate our approach in steady-state configurations, demonstrating numerical con- vergence rates. In particular, we achieve second-order accuracy for the Dirichlet boundary case. Unlike [2], our formulation explicitly includes the term γn, which accounts for ion- ization effects in plasma modeling. We then extend our analysis to time-dependent cases,

∂F



(a) Primal mesh M (b) Dual mesh M^*

Figure 1: Example of the primal and dual meshes when a quadrangular grid is considered. The circle corresponds to the primal unknowns while the square indicates the dual ones. The filling indicates boundary unknowns.

testing various time discretization schemes, including explicit and implicit Euler methods, as well as a θ-scheme.

This study highlights the potential of diamond-based schemes, such as DDFV, for solving multi-scale and multi-physics problems involving coupled equations. Our proposed self-consistent DDFV scheme for the convection-diffusion equation can be naturally combined with the Poisson solver from [1], providing a unified framework for cold plasma modeling.

Acknowledgment

The authors would like to thank the "GDR Emili" for the support of the collaboration between the authors.

References

[1] T. Bonnafont, D. Bessi`eres, J. Paillol. 2024. A finite volume method to solve the Poisson equation with jump conditions and surface charges: Application to electroporation. Journal of Computational Physics. Vol. 504, pp. 112862.

[2] Y. Coudi`ere, G. Manzini. 2010. The discrete dual finite volume method for convection-diffusion problems. SIAM Journal on Numerical Analysis. Vol. 47, pp. 4163-4192.

[3] D. Bessi`eres, J. Paillol, A. Bourdon, P. S´egur, E. Marode. 2007. A new one-dimensional moving mesh method applied to the simulation of stramer discharges. Journal of Physics D: Applied Physics. Vol. 40, pp 6559.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Modelling of Bubble Breakage and Coalescence in Stirred and Sparged Bioreactor Using the Euler-Lagrange Approach Coupled with VOF

P. Kry´sa[1,2,*], S. Kuhn[2], M. S˘o´o˘s[1]

[1] Department of Chemical Engineering, University of Chemistry and Technology Prague, Technick´a 3, 166 28 Prague 6, Czechia, e-mail: krysap@vscht.cz

[2] Department of Chemical Engineering, KU Leuven, Celestijnenlaan 200F, 3001 Leuven, Belgium

Abstract: Efficient mass transfer is critical for stirred and sparged bioreactors used in cell culture and the production of high-value biopharmaceuticals. Accurate prediction of volumetric mass transfer coefficient k_La requires modelling of not only the dispersed bubbles but also the free surface. To achieve this, we developed an Euler-Lagrange (EL) model coupled with the Volume of Fluid (VOF) method, which allowed us to account for free surface dynamics and its contribution to the total k_La, which is often overlooked. Continuous phases (water and air above the free surface) were calculated using the Reynolds-averaged Navier-Stokes (RANS) method together with realizable k-ε turbulence model. The motion of the Lagrangian dispersed bubbles was done by integration of Newton's equation of motion. Since the correct prediction of k_La depends on the bubble size, we accounted for bubble breakage [1, 2, 3] and coalescence [3, 4, 5, 6] as well as shape deformation caused by turbulence. Two vessels (250 mL and 3.5 L) under various impeller speeds (972 rpm and 200, 350 and 500 rpm) and constant gas feed rates (0.133

and 0.33 vvm) for each vessel were simulated. Then, the outputs were validated against experimental data, focusing on both bubble sizes and volumetric mass transfer coefficient, where we obtained very nice agreement of predicted and experimental values. Additionally, we tested and evaluated the influence of additional forces on the resulting mean Sauter diameter d_{32}, void fraction and k_La. We observed increase in void fraction (and thus also interfacial area and k_La) if pressure gradient force (PGF) was included. This occurred by slowing the bubbles down without significatly altering the d_{32}. The free surface contribution [7] to overall k_La appears to be important and comparable to the one of sparged bubbles, particularly in small-scale reactors and at very low gas flow rates. As a result of these advancements, our EL-VOF model provides a comprehensive and reliable framework for simulating gas-liquid systems. It enables accurate predictions of bubble behaviour, size distribution and interactions with the liquid phase and it effects on mass transfer.

Keywords: CFD, multiphase, Euler-Lagrange, VOF, bubbles, breakage, coalescence

---

* Presenting author

References

[1] C. Mart´ınez-Baz´an, J. L. Montan˜´es, J. C. Lasheras, On the breakup of an air bubble injected into a fully developed turbulent flow. Part 1. Breakup frequency, Journal of Fluid Mechanics 401 (1999) 157–182. doi:10.1017/S0022112099006680.

[2] C. Mart´ınez-Baz´an, J. L. Montan˜´es, J. C. Lasheras, On the breakup of an air bubble injected into a fully developed turbulent flow. Part 2. Size PDF of the resulting daughter bubbles, Journal of Fluid Mechanics 401 (1999) 183–207. doi:10.1017/S0022112099006692

[3] P. Kry´sa, M. Sˇo´oˇs, Modelling of bubble breakage and coalescence in stirred and sparged bioreactor using the euler-lagrange approach, International Journal of Heat and Mass Transfer 199 (2022) 123466. doi:10.1016/j.ijheatmasstransfer.2022.123466.

[4] M. J. Prince, H. W. Blanch, Bubble coalescence and break-up in air-sparged bubble columns, AIChE Journal 36 (1990) 1485–1499. doi:10.1002/aic.690361004.

[5] M. Sommerfeld, Validation of a stochastic lagrangian modelling approach for inter-particle collisions in homogeneous isotropic turbulence, International Journal of Multiphase Flow 27 (2001) 1829–1858. doi:10.1016/S0301-9322(01)00035-0

[6] R. Sungkorn, J. J. Derksen, J. G. Khinast, Euler-lagrange modeling of a gas-liquid stirred reac- tor with consideration of bubble breakage and coalescence, AIChE Journal 58 (2012) 1356–1370. doi:10.1002/aic.12690

[7] F. O¨ zkan, A. Wenka, E. Hansjosten, P. Pfeifer, B. Kraushaar-Czarnetzki, Numerical investigation of interfacial mass transfer in two phase flows using the vof method, Engineering Applications of Compu- tational Fluid Mechanics 10 (2016) 100–110. doi:10.1080/19942060.2015.1061555

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Scalar Mixing Characteristics of an Elevated Low Velocity Ratio Jet in Atmospheric Crossflow using IDDES

Ilyas Yilmaz*

Dept. of Mechanical Engineering, Fac. of Engineering and Natural Sciences, Istanbul Bilgi University, 34060, Eyupsultan, Istanbul, Turkiye, E-mail: ilyas.yilmaz@bilgi.edu.tr

Abstract:

Scalar mixing characteristics of an elevated low velocity ratio jet flowing into atmospheric crossflow are studied using Improved Delayed Detached Eddy Simulation (IDDES) implemented in OpenFOAM.

A realistic configuration, which in practice may be relevant to a jet issuing from a power plant chimney into atmosphere, is considered. This scenario is particularly important for Environmental Engineering issues.

First, formation and development of large scale coherent turbulent flow structures (ie, Kelvin-Helmholtz roll-up, Counter-rotating vortex pair, Omega-shape vortices, Horse shoe vortex and Hairpin vortices) in the transitional regime, where jet-to-crossflow velocity ratio is low, are identified. It is shown that IDDES can predict flow field with a reasonable accuracy on adequately generated moderate grids with proper use of wall functions.

Then, influence of jet inlet turbulence intensity on scalar mixing dynamics is investigated. It is observed that formation and evolution of the large scale coherent flow structures in

the wake are determined by the jet inlet turbulence level, and scalar mixing and dissipation mostly follow the spatial and temporal patterns of these structures, which becomes more apparent at high turbulent intensities at jet inlet.

Results also reveal that strength of counter-rotating vortex pair decreases with increasing jet inlet turbulence level, leading to faster breakdown. This enhances scalar mixing in near-wake region and along the jet trajectory, characterized by faster spreading rate and diffusion, and wider mixing zone especially in lateral directions.

Detailed mechanism of scalar mixing dynamics for the given scenario will be described in the manuscript using various qualitative and quantitative analyses.

Keywords: Jet in atmospheric crossflow, Scalar mixing, Low velocity ratio jet, Elevated jet, Improved Delayed Detached Eddy Simulation (IDDES)

---

* Presenting author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Alleviating Spurious Wave Reflection with Filters, Absorbing Layers and Artificial Neural Network Couplings

K. F. CHAN[1,*], N. BOMBACE[2], S. FALCO[1], D. WASON[1], T. WELSCH[1], D. CHAPMAN[1],

N. PETRINIC[1], AND D. EAKINS[1]

[1] Impact and Shock Mechanics Laboratory, Department of Engineering Science, University of Oxford,

Parks Road, Oxford, OX1 3PJ, UK

[2] Adaptive, Embedded and AI (AEAI) Group, Advanced Micro Devices Inc., Darwin House,

Edinburgh Technopole, Bush Estate, EH26 0PY Edinburgh, UK

Keywords: Spurious Wave Reflection, Multi-Time Stepping, Perfectly Matched Layer

---

* Presenting author

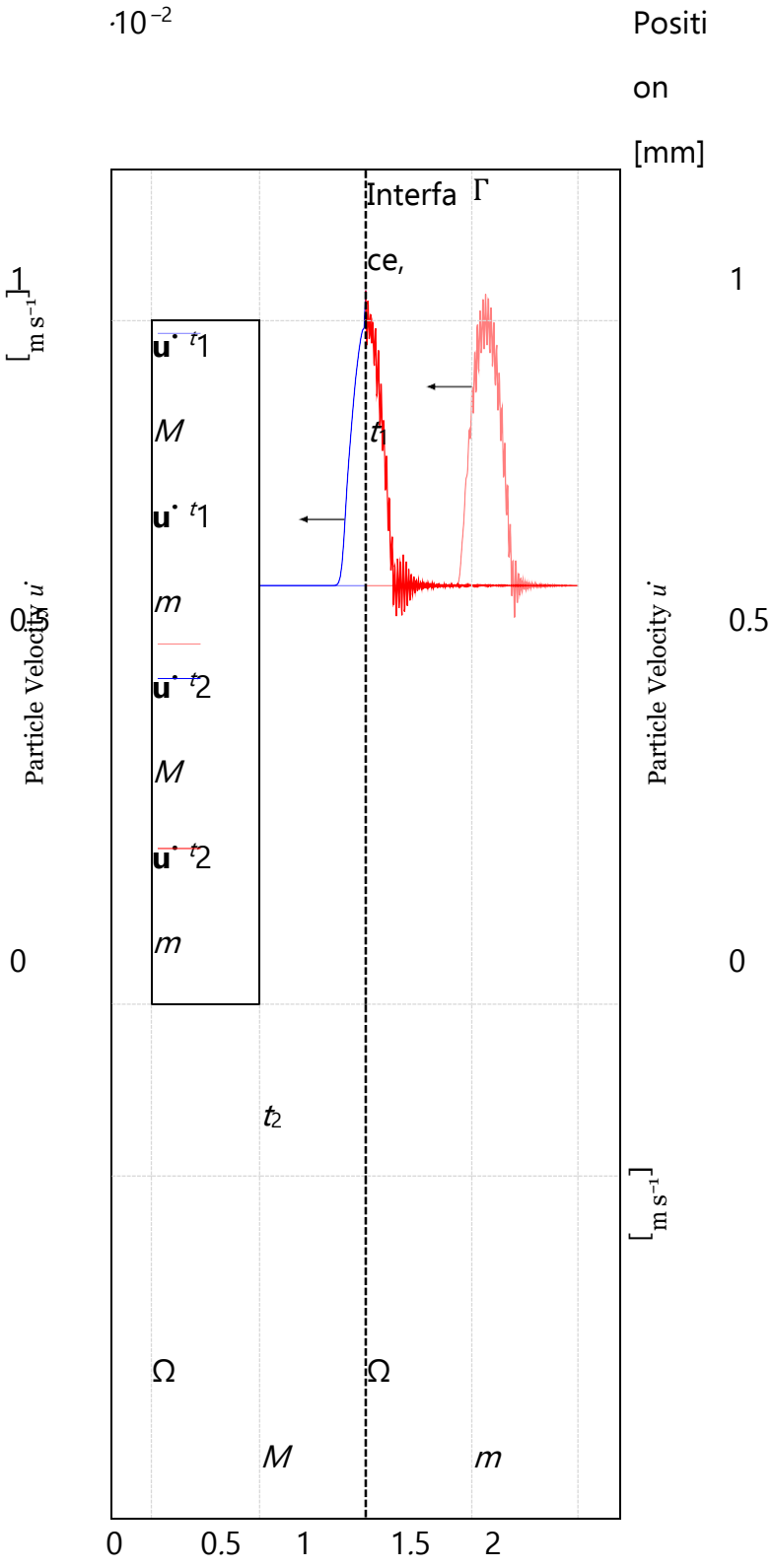
Accurate simulation of high-frequency stress wave propagation through multi-scale systems presents significant obstacles, particularly when coupling micro- and macro-scale finite ele- ment (FE) domains. The disparity in mesh sizes across these domains often lead to spurious wave reflections at the interfaces, generating numerical artifacts that

compromise the relia- bility of predictions [1]. In Figure 1, the superposition of two frequencies is shown, where reflection back into the micro-domain is generated. This approach is also applicable to het- erogeneous domains with non-matching meshes across spatial scales [2]. This study provides a systematic comparison of three distinct approaches - filtering methods, absorbing layers, and artificial neural networks (ANNs) to mitigate these artifacts and improve the fidelity of coupled multi-scale simulations.

Firstly, we examine filtering techniques, including the application of corrective kinematic boundary conditions, which act on the solution to remove high-frequency numerical noise. These methods offer direct control over spurious components but may introduce numerical dissipation that alter wave amplitudes. Next, we evaluate absorbing layers, in the form of Perfectly Matched Layers (PML) which function by gradually dampening incompatible waves at the interfaces of macro- and micro-domain. While effective in preventing wave reflections, these methods require careful parameter tuning and additional computational overhead. Finally, we investigate the use of artificial neural networks (ANNs) trained to learn and correct spurious reflections at the interface. By analysing wave transmission and reflection patterns from high-fidelity micro simulations, ANNs provide a data-driven mechanism that adapts to different coupling conditions.

Additionally, we incorporate a multi-time stepping strategy to enhance the computational efficiency, allowing macro and micro elements to integrate with their own respective time step [3]. Leveraging several time steps in a domain permits explicit time integration close to the Courant-Friedrichs-Lewy (CFL) condition in each domain, as well as fewer steps com- pared to state-of-the-art asynchronous integration methods. The direct solution of interface conditions ensures the continuity of tractions and accelerations for a variety of

heteroge- neous configurations. The combination of spurious wave correction and multi-time stepping produce solutions with fewer numerical artifacts and lower runtimes.


·10 −2
Positi
on
[mm]
Interfa
ce,
Γ
1
[m s−1]
0.5
Particle Velocity u
0
u· t1
M
u· t1
m
u· t2
M
u· t2
m
t1
t2
Ω
Ω
M
m
0
0.5
1
1.5
2
1
0.5
Particle Velocity u
0
[m s−1]

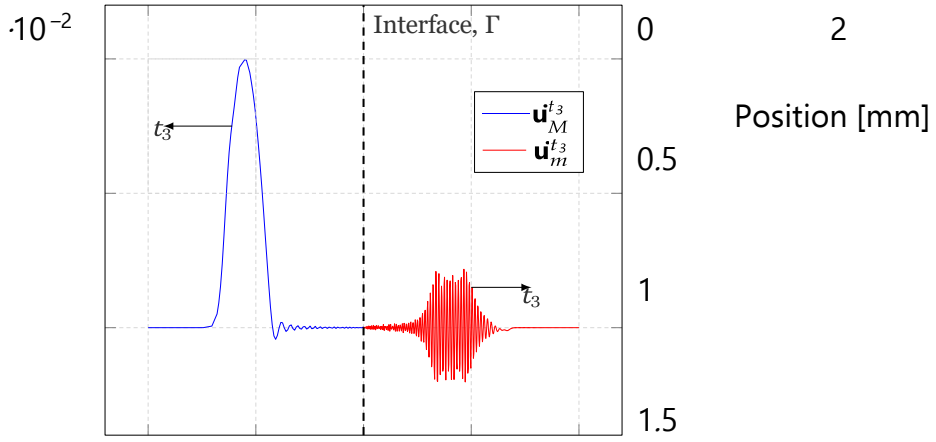


Figure 1: The problem of spurious wave reflection generated from the interaction of a high frequency stress wave travelling from micro (Ω_m) to macro (Ω_M) domain with mesh sizes of 0.002 and 0.008 mm, respectively.

The effectiveness of filtering, absorbing layers, and ANNs is assessed using benchmark prob- lems involving a variety of high-frequency wave transmissions across disparate finite element meshes. Key performance metrics include reflection coefficients, conservation of energy, computational cost, and robustness to varying interface conditions. Preliminary results in- dicate that filtering techniques effectively reduce spurious reflections but may lead to slight amplitude loss. Absorbing layers provide strong reflection suppression but are sensitive to parameter selection and increase computational cost. ANNs demonstrate promising ac- curacy by adapting to complex wave interactions but require extensive training data and computational resources for implementation. This work highlights the

trade-offs between these methods, unveiling the correct selection of mitigating method depending on accuracy, efficiency, and ease of implementation.

References

[1] Grunwald, C., Sauer, M., Stolz, A. and Hiermaier, S., 2025. Enhancing Efficiency in Multiscale Simulation: Comparing a Lagrange Multiplier Based Approach and a Weak Staggered Coupling With Optional SPML Interface for Wave Propagation. International Journal for Numerical Methods in Engineering, p.e7633.

[2] Chan, K.F., Bombace, N., Sahu, I., Falco, S. and Petrinic, N., 2025. Temporal and Spatial Coupling Methods for the Efficient Modelling of Dynamic Solids. Materials, inRev.

[3] Chan, K.F., Bombace, N., Sap, D., Wason, D., Falco, S. and Petrinic, N., 2025. A Multi-Time Stepping Algorithm for the Modelling of Heterogeneous Structures With Explicit Time Integration. International Journal for Numerical Methods in Engineering, Vol. 126(1), pp.e7638.

The Onsager principle as an approximation tool in multi-physics multi-scale problem

Xianmin Xu 1,a

[1] AMSS, Chinese Academy of Sciences, E-mail: xmxu@lsec.cc.ac.cn

The Onsager principle is a fundamental law for irreversible processes in statistic physics. It has been used to develop mathematical models for many dissipative systems in soft matter, like colloid solution, liquid crystal and the moving contact line problem, etc. Recently, the variational principle has been used as an approximation tool to derive reduced models. In this talk, I will talk some recent progress in this field. We will show that the principle can be generalized to model non-isothermal multi-phase fluid with inertial effect and problems with non-quadratic dissipations. This helps us to develop reduced models and efficient numerical methods for complicated multiscale multiphysics phenomena.

Keywords:

Onsager principle, Model Reduction, multiphase flow, multiscale, Multiphysics,

[a] Presenting Author

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

Dynamics of charged particles in low-Reynolds-number fluids confined in general geometries

Zhuang Sun [1,2], Juan J. de Pablo [3,4], Xikai Jiang [1,2,a]

[1] Institute of Mechanics, Chinese Academy of Sciences, E-mail: xikaij@imech.ac.cn

[2] School of Engineering Sciences, University of Chinese Academy of Sciences

[3] University of Chicago, E-mail: depablo@uchicago.edu

[4] Materials Science Division, Argonne National Laboratory

A scalable parallel computational framework is developed for description of hydrodynamic and electrostatic interactions between particles in low-Reynolds-number fluids confined in general geometries. The general geometry Stokeslet is calculated following a matrix-free algorithm using the general geometry Ewald-like method. The electrostatics considers dielectric mismatch between different materials in the computational domain, and a boundary element method accelerated by a fast multiple method is used to solve the electrostatic problem. We illustrate applications of the computational approach in the context of the dynamics of confined charged particles under non-equilibrium conditions. Acknowledgement: this work was supported by the International Cooperation Grant from Chinese Academy of Sciences (No. 025GJHZ2022023MI).

Keywords:

Particle dynamics, low-Reynolds-number fluid, hydrodynamic interaction, electrostatic interaction

[a] Presenting Author

References:

[1] X. Zhao, J. Li, X. Jiang, D. Karpeev, O. Heinonen, B. Smith, J. P. Hernandez-Ortiz, and Juan J. de Pablo 2017 Parallel O(N) Stokes' solver towards scalable Brownian dynamics of hydrodynamically interacting objects in general geometries, J. Chem. Phys., 146: 244114

[2] J. Li, X. Jiang, A. Singh, O. Heinonen, J. P. Hernandez-Ortiz, and Juan J. de Pablo 2020 Structure and dynamics of hydrodynamically interacting finite-size Brownian particles in a spherical cavity: spheres and cylinders. J. Chem. Phys., 152: 204109

[3] Z. Sun, G. Chen, Juan J. de Pablo, and X. Jiang 2024 Particulate transport in the low- reynolds-number fluid confined in a spherical cavity. Chinese J. Theor. Appl. Mech., 56: 1-13

[4] G. Chen, X. Jiang 2023 Single-particle dynamics in a low-Reynolds-number fluid under spherical confinement. J. Fluid Mech., 969: A

Discrete-to-Continuum Computational Homogenization of Lattice Materials

ALESSANDRA PAOLONI[1,*], CRISTINA GATTA[1], ELIO SACCO[2], DANIELA ADDESSI[1]

[1] Sapienza University of Rome, E-mail: alessandra.paoloni@uniroma1.it,cristina.gatta@uniroma1.it,daniela.addessi@uniroma1.it

[2] University of Naples Federico II, E-mail: elio.sacco@unina.it

Abstract: In recent years, architected materials have received great attention, as they manifest special engineering properties that conventional materials do not exhibit, such as: negative Poisson's ratio, high strength-to-weight ratio, high energy absorption capabilities, as well as designed band-gaps [1]. These ma- terials, also known as metamaterials, are often obtained by tessellation of unit cells, which can be composed of beam-like elements consitituting lattice materials. Therefore, they represent an ideal candidate to be an- alyzed through the consolidate techniques usually employed for periodic media, such as the homogenization approach [2]. The latter allows to determine the average mechanical properties of the real discrete medium through the study of a small portion of it.

Relying on the above considerations, this study presents a computational homogenization procedure to an- alyze the behavior of periodic lattices. Following a two-scales approach, the lattice structure is modeled at two scales: the macroscopic structural level

(macroscale), where the real medium is substituted by an equivalent fictitious homogeneous continuum, and the microscopic material level (microscale), where a representative volume element (RVE) of the material is properly selected accounting for all the details about the microstructure. According to the strain driven formulation, the developed homogenization procedure involves a downscaling process based on the definition of a kinematic map that relates the microscale dis- placements to the macroscale deformations. At the microscale, an enhanced beam formulation is adopted for each element composing the RVE. Finally, the Hill-Mandel condition is invoked to evaluate the homogenized stresses and constitutive operator and to perform the upscaling.

The overall procedure is validated through the simulation of examples available in the literature [3], also considering various lattice topologies. Moreover, comparisons between results derived from the proposed multiscale model and those recovered by detailed micromechanical analyses are given, thus proving the accuracy of the homogenized solutions as well as the advantages of the multiscale procedure in terms of computational burden.

Keywords: Computational homogenization, lattice material, representative volume element, discrete-to- continuum

---

* Presenting author

References

[1] X. Zheng, H. Lee, T.H. Weisgraber, et al. 2014. Ultralight, ultrastiff mechanical meta-materials. Science; Vol. 344(6190), pp. 1373-1377.

[2] J. Somnic, W.J. 2022. Status and challenges in homogenization methods for lattice materials. Materials 15.2: 605.

[3] A. Vigliotti, D. Pasini. 2012. Linear multiscale analysis and finite element validation of stretching and bending dominated lattice materials. Mechanics of Materials, Vol. 46, pp. 57-68.

Lithium Nanoparticle Dynamics in Flame Spray Pyrolysis: From Evaporation, Decompostion to Agglomeration

Ruitian He[1,a], Kai H. Luo[2,*]

[1] University College London, E-mail: ruitian@ucl.ac.uk

[2] University College London, E-mail: k.luo@ucl.ac.uk

Flame spray pyrolysis (FSP) has emerged as an industrially scalable and versatile technique, which paves the way for one-step synthesis of various nanomaterials, with applications in batteries, gas sensors, environmental treatment, etc. However, the properties and performance of nanomaterials produced depend on complex interactions among multi-physics processes in FSP, including liquid atomization, droplet evaporation, precursor decomposition/oxidation, and subsequent nanoparticles nucleation and agglomeration. Many efforts have been devoted to understanding the mechanisms of the above processes and to elucidating key control parameters, using optical/sampling diagnostics and numerical simulation methods. Generally, the precursor droplet size is regarded as one of the most important control factors in FSP, as it is directly linked to the atomization quality, affecting the high-temperature residence time and nanoparticles growth rate. Nevertheless, in-depth insight into how the precursor droplet size affects the nanoparticle products remains unclear, which hinders further optimization of the FSP process.

This study has unravelled the role of precursor droplet size behinds the multi-physics evolution of lithium nanoparticles in FSP. A series of reactive molecular dynamics (MD) simulations for a single lithium precursor droplet with various initial diameters, has been performed. Comprehensive analyses of the droplet's morphology and energy evolution, bond kinetics, atomic motion, gas

decomposition and synthesized lithium nanoparticles are conducted, as shown in Figure 1. It is found that gas accumulation plays a dominant role in shaping the droplet's morphological characteristics throughout its lifetime, as indicated by the continuously expanding droplet's volume and the formation of a hollow structure. As the initial size of precursor droplet increases, despite more decomposed gas is trapped inside the droplet, the explosion behaviour becomes less intense because of the reduced fraction of decomposed gas within the droplet. Furthermore, with the increasing initial droplet size, more lithium atoms tend to agglomerate to generate lithium nanoparticles with greater size, as evidenced by the increased normalized lithium bonds and slower atomic motion. Nevertheless, this size effect becomes less pronounced for the fine-sized nanoparticles formation in the later heating up period.

Keywords:

Lithium Nanoparticles, Flame Spray Pyrolysis, Precursor Droplet Size, Reactive Molecular Dynamics, Multi-physics Processes

[a] Presenting Author

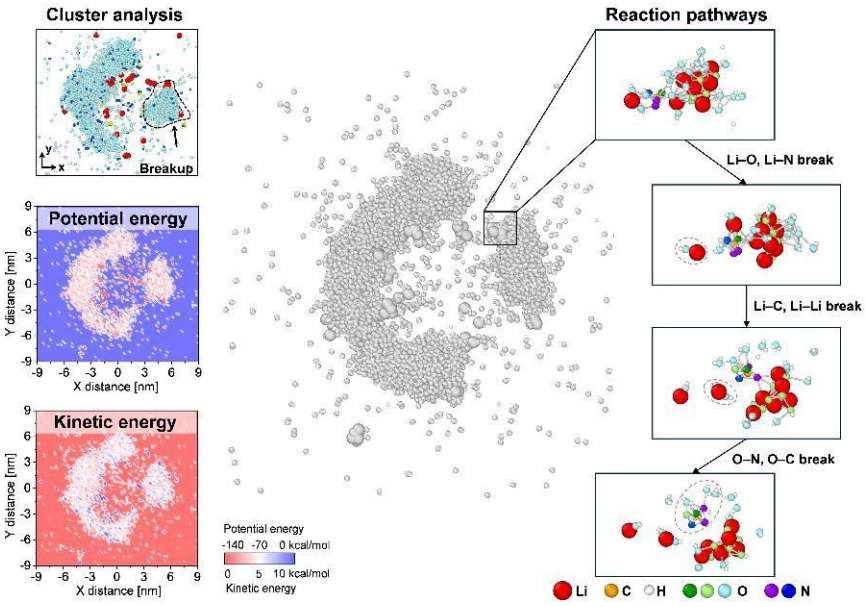


Figure 1. Reactive molecular dynamics simulation of a lithium precursor droplet under flame spray pyrolysis-like conditions

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Efficient multiscale simulations of additively manufactured alloys: Toward a hybrid approach combining FE^2 and FE-NN

A. RADERMECKER[1,*], Prof. A. SIMAR[2] and Prof. J.-P. PONTHOT[3]

[1]University of Li`ege, Belgium, E-mail: arnaud.radermecker@uliege.be [2]University of Louvain, Belgium, E-mail: aude.simar@uclouvain.be [3]University of Li`ege, Belgium, E-mail: jp.ponthot@uliege.be

Abstract: Metafor [1], our in-house nonlinear finite element software, is now capable of efficiently performing both 2D and 3D finite element squared (FE^2) [2] simulations, as illustrated in Fig. 1. This efficiency is achieved through several optimisations, including the parallelisation of microscale finite element analyses, the

computation of macroscopic tangent moduli via static condensation of the microscale Representative Volume Element (RVE) using only two nodes in 2D or three nodes in 3D, and various numerical enhancements.

However, despite these improvements, the inherent computational cost of FE^2 remains a significant challenge for multiscale simulations.

In recent years, neural networks (NNs) have gained popularity as surrogates for microscale simulations, giving rise to the FE-NN paradigm as an alternative to conventional FE^2

approaches. While this method enables significantly faster online computations, it entails high offline costs associated with data generation and model

training. Moreover, the accuracy of NNs is inherently limited to their training data, posing challenges in path-dependent microstructures, where all possible loading paths must therefore be considered. These paths are often generated using stochastic methods, such as random-walk algorithms, making it difficult for users to obtain a clear understanding of the dataset. Additionally, the reliance on complex NN architectures, such as recurrent neural networks (RNNs), gated recurrent units (GRUs), or long short-term memory networks (LSTMs), further increases training costs.

To address these challenges, we propose a novel hybrid approach that combines the efficiency of FE-NN with the accuracy of FE^2. Rather than relying solely on a complex NN architecture, a simpler model, such as a feedforward neural network, can be utilised. Trained on a well-defined dataset of path-dependent microscale simulations, this NN efficiently predicts responses for known loading scenarios at a fraction of the computational cost. When an unseen loading path is encountered, the code dynamically switches from the NN to a classical finite element analysis of the microstructure, thereby transitioning from FE-NN to FE^2. Fig. 2 presents a preliminary proof of concept.

This transition occurs independently at each Gauss point of the macroscale, allowing the multiscale simula- tion to maintain overall efficiency while ensuring that the neural network operates within its trained range. As a result, most of the macroscale domain benefits from the NN's speed, while only critical regions tran- sition to a classical finite element analysis when the NN lacks accuracy. This strategy provides an optimal balance

between computational efficiency—both in offline and online phases—and numerical precision.

Furthermore, while optimising computational cost, this strategy also enables users to analyse the microstruc- tural response in critical regions where the transition to classical finite element analysis has occurred, thereby providing deeper insights into the material's microscale behaviour.

Keywords: finite element squared, neural networks, multiscale simulations

---

* Presenting author

References

[1] MN2L Uli`ege Non-Linear Computational Mechanics Laboratory. Metafor, an object-oriented finite element code for the simulation of solids submitted to large deformations, 2025. http://metafor.ltas.ulg.ac.be/.

[2] M. G. D. Geers, V. G. Kouznetsova, and W. A. M. Brekelmans. *Computational homogeniza- tion*, volume 522 of *CISM International Centre for Mechanical Sciences*, page 327–394. Springer Vienna, Vienna, 2010.

[3] Ling Wu and Ludovic Noels. Self-consistency reinforced minimal gated recurrent unit for surrogate modeling of history-dependent non-linear problems: Application to history- dependent homogenized response of heterogeneous materials. *Computer Methods in Applied Mechanics and Engineering*, 424:116881, May 2024.

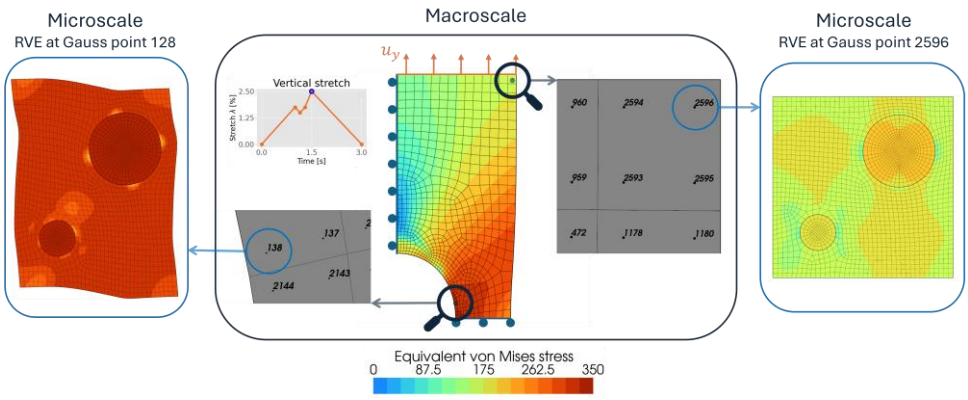


Figure 1: FE^2 simulation result from Metafor. This simulation is inspired by [3]. It includes 2,640 macro Gauss points and 116 computed steps, resulting in a total of 165 Newton-Raphson iterations. The RVE consists of elastic particles embedded in an elasto-plastic matrix. This Metafor FE^2 simulation took 1h50 on 64 cores, equivalent to 173 CPU-hours, and was 153 times faster than [3].

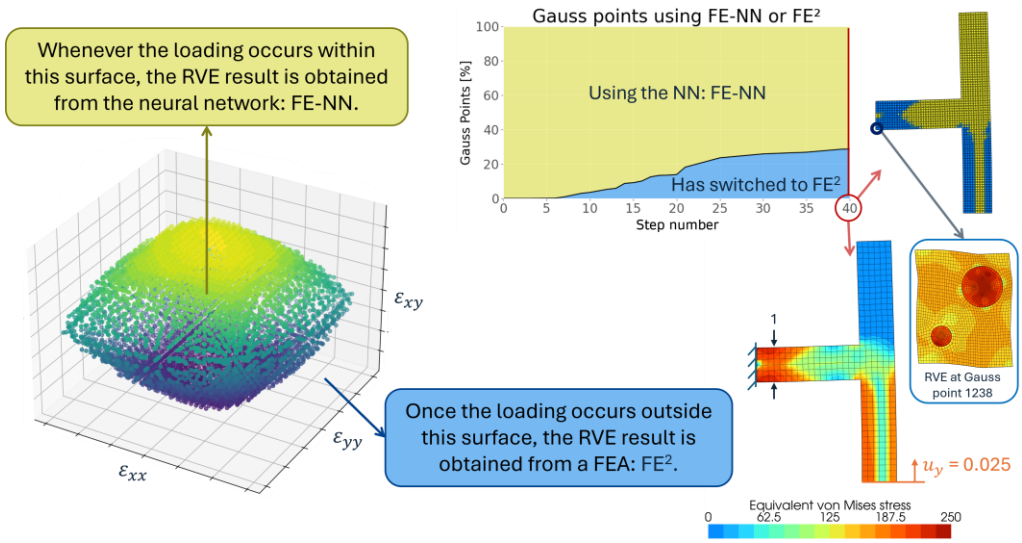


Figure 2: First proof of concept of the hybrid FE-NN and FE^2 method in Metafor. In this initial validation, the neural network emulates the elastic response of the RVE shown in Fig. 1.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Phase-field Model for Multiple Phases and Grains using Finite Difference Method

Dong-hwa Lee [a], Hyochan Kim

Korea Atomic Energy Research Institute, E-mail: donghwalee@kaeri.re.kr

Over the past two decades, the phase-field model has become one of the most widely used methods for simulating microstructure evolution, such as grain boundary migration, dendrite formation, spinodal decomposition, and phase separation.

Among various phase-field-based grain growth models, the most commonly applied approach [1] employs a set of non-conserved order parameter fields to define grain domains. In this model, the local energy at interfaces is set higher than within the grains, generating a thermodynamic driving force that minimizes interfacial energy while reducing the system's total energy.

In this study, a phase-field-based grain growth model is developed to investigate multi- phase materials. The governing equation is formulated using the Allen-Cahn equation, with a set of field variables and order parameters evolving over space and time. The model accommodates NN possible phases and KK possible chemical species [2], allowing for distinct interfacial energies between grains and phases. The formulation is discretized in space and time, and an implicit Euler scheme is implemented using the finite difference method for simplicity.

To verify the model, an ideal spherical grain growth simulation was conducted. The grain retained its spherical shape while shrinking, demonstrating the expected behavior. Additionally, for multi-phase grain growth verification, a binary alloy system was used to model an allotriomorph. A circular α grain was initially placed between two β grains. By applying appropriate parameters from [2], we observed that the circular

grain transformed into a lenticular shape with the theoretically predicted dihedral angle.

Keywords:

phase-field model, grain growth simulation, multiple phases, multiple grains

---

[a] Presenting Author

References:

[1] Chen, L. Q., & Yang, W. (1994). Computer simulation of the domain dynamics of a quenched system with a large number of non-conserved order parameters: The grain-growth kinetics. Physical Review B, 50(21), 15752.

[2] Aagesen, L. K., Gao, Y., Schwen, D., & Ahmed, K. (2018). Grand-potential-based phase- field model for multiple phases, grains, and chemical components. Physical Review E, 98(2), 023309.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Post-buckling and nonlinear thermal stress of laminated composite by CUF

F. Bracaglia [1,a] , A. Pagani[2], E. Zappino[3] E. Carrera[4]

[1] Mul2 Lab, DIMEAS, Politecnico di Torino, Corso Duca degli Abruzzi 24, Torino , Italy.

E-mail: francesca.bracaglia@polito.it

[2] Mul2 Lab, DIMEAS, Politecnico di Torino, Corso Duca degli Abruzzi 24, Torino , Italy.

E-mail: alfonso.pagani@polito.it

[3] Mul2 Lab, DIMEAS, Politecnico di Torino, Corso Duca degli Abruzzi 24, Torino , Italy.

E-mail: enrico.zappino@polito.it

[4] Mul2 Lab, DIMEAS, Politecnico di Torino, Corso Duca degli Abruzzi 24, Torino , Italy.

E-mail: erasmo.carrera@polito.it

Advanced composite materials offer high specific stiffness and strength and a nearly zero coefficient of thermal expansion in the fiber direction, making them suitable for extreme thermal environments [1]. When high temperatures are reached, a thermo-elastic linear analysis is no longer sufficient to describe the structural behavior. Furthermore, the thermal load acts as a volume force affecting both the displacement and stress fields.

It is well known that, once a specific value of overtemperature has been reached, it is no longer possible to restrict the structural description to small displacements and rotations. In such cases, the introduction of a nonlinear geometrical relation becomes imperative, particularly for highly flexible structures.

Large deformations result in coupled bending, torsion, shear, and membrane behavior, which in turn leads to high nonlinear phenomena [1,2]. Post-buckling behavior and high deflection description of structures under mechanical field have been vastly investigated [3,4], and analogous considerations must be done for thermal loading.

The study centers on the description of the thermal post-buckling behavior of composite structures with a particular focus on high-displacement levels and consequent stress fields. The governing equations are derived from the Principle of Virtual Displacement (PVD), where the nonlinearities are incorporated through the full Green-Lagrange strain tensor. The structural model is obtained through the Finite Element Method (FEM), where high-order theories are implemented within the Carrera Unified Formulation (CUF) [5]. The nonlinear problem is solved using the Newton-Raphson method combined with the arc-length constraint. The thermal load is applied uniformly across the thickness. Furthermore, it is analyzed through a decoupled approach, where the thermal profile is assumed to be known and is treated as an external load.

The results show the influence of the adopted expansion theory in their accuracy and the necessity of using these models combined with the nonlinear description to accurate predict the displacement and stresses field. Different geometries and materials are evaluated, and the

[a] Presenting Author

importance of the nonlinear terms in the buckling investigation is assessed. Post-buckling configuration is described and secondary buckling deflection are also investigated.

Keywords: Finite element method, nonlinear buckling, nonlinear thermal stress, thermos- elastic analysis, geometrically nonlinear.

References:

[1] A. K. Noor and W. S. Burton. Computational models for high-temperature multilayered composite plates and shells. Applied Mechanics Reviews, 45(10):419–446, October 1992.

[2] M. Sathyamoorthy. Nonlinear analysis of structures. Mechanical engineering series. CRC, Boca Raton, 2017.

[3] C. Y. Chia. Geometrically nonlinear behavior of composite plates: A review. Applied Mechanics Reviews, 41(12):439–451, December 1988.

[4] A. Pagani, P. Chiaia, and E. Carrera. Vibration of solid and thin-walled slender structures made of soft materials by high-order beam finite elements. International Journal of Non-Linear Mechanics, 160:104634, April 2024.

[5] E. Carrera, E. Zappino, M. Cinefra, and M. Petrolo. Finite element analysis of structures through unified formulation. Wiley, Chichester, West Sussex, 2014.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Leveraging Full-field Meso-scale Models of Polycrystalline Materials to Hierachically Propogate High-rate Inter-granular Fracture Mechanics to Macro-scale Models

D. WASON [1,i], S. FALCO [1], L. SMITH[1], D. EAKINS[1]

[1] Impact and Shock Mechanics Laboratory, Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, UK,

E-mail: david.wason@eng.ox.ac.uk

Keywords:

High-rate loading, Polycrystalline materials, Intergranular cracking, Crystal plasticity-based finite element modelling (CPFEM), Explicit user subroutine, Multi-scale modelling, Stochastic modelling, Hierarchical modelling

[i] Presenting Author

The early stages of fracture in high-rate-loaded polycrystalline materials are typically highly localised and originate from intra- and inter-granular mechanisms. Characterisation of crack initiation locations for AZ31B-O found that inter-granular cracking comprised > 57.2 % of those observed for various rolling direction orientated load cases, with the rest being trans- granular [1]. The accurate simulation of such phenomena using finite element modelling approaches require a relatively fine discretisation when compared to those used when modelling high-rate industrial and practical events, so much so the wholesale utilisation of such a fine mesh would be prohibitively expensive to run, even with recent advances in computing power.

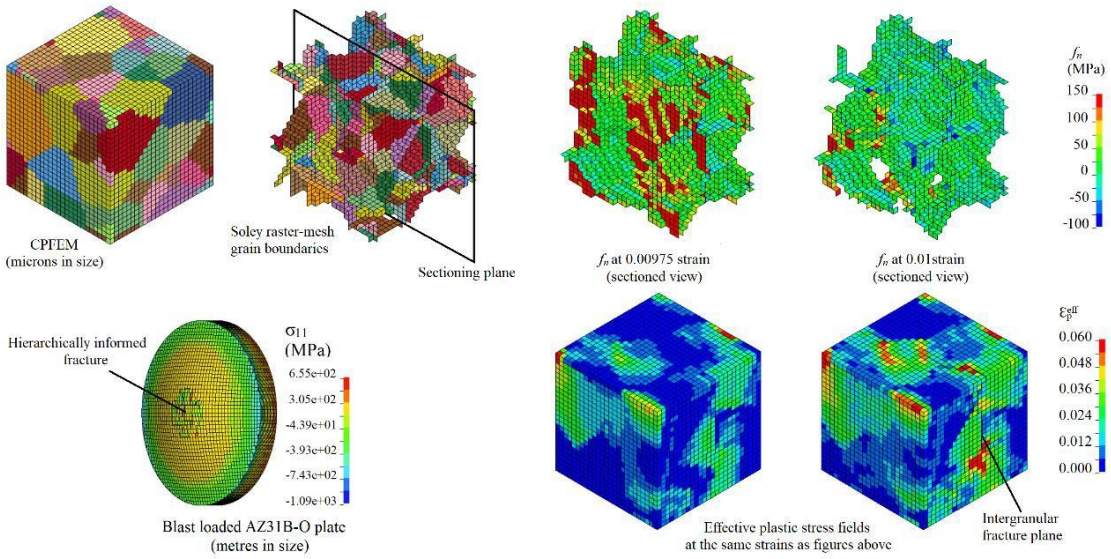


Figure 1: Sample of graphics presenting key features from this work. (Top left) Example of CPFEM and corresponding raster-mesh grain boundaries, (Top right) Stress relaxation associated with grain boundary fracture, (Bottom right) Strain localization and associated fracture, (Bottom left) Example of hierarchically informed fracture.

In this work, a full-field homogenisation scheme [2] that utilises an explicit crystal plasticity-based user subroutine that considers twinning through volume fractions, for improved efficiency, is coupled with an inter-granular cracking user subroutine [3], to model the observed dominant fracture mechanism in AZ31B-O subjected to high-rate loading (see Figure 1). As the polycrystalline generating algorithm used inherently introduces variability, the resulting uncertainty in fracture characteristics can be quantified through use of the representative volume element-sized crystal plasticity-based finite element models generated as part of the homogenisation scheme. With the characterisation of a sufficiently large number of these models to constitute a distribution, with large numbers of models being run in parallel batches on a high-performance cluster, the resulting parameter space can be used to stochastically inform a macro-scale model, hierarchically. Finally, the models provide insight into how variations in meso-scale properties influence fracture behaviour (e.g. grain size distribution, critical resolved shear stresses, grain boundary strength).

References:

[1] Jamali, A. Ma, and J. LLorca. "Influence of grain size and grain boundary misorientation on the fatigue crack initiation mechanisms of textured AZ31 Mg alloy". In: *Scripta Materialia* **207** p. 114304 (2022).

[2] Wason, D. "A Multi-scale Approach to the Development of High-rate-based Microstructure-aware Constitutive Models for Magnesium Alloys". PhD thesis. University of Oxford, 2024.

[3] Falco, S., Fogell, N., Iannucci, L. *et al.* "Raster approach to modelling the failure of arbitrarily inclined interfaces with structured meshes". In: *Comput Mech* **74**, 805–818 (2024).

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Numerical Modeling of Gas Release from Underground Gas Hydrates and Its Upward Movement taking into account the Nonlinearity of the Filtration Law A

HMED BAKEER [1,a], GRIGORY KAZAKEVICH[2], YURY POVESHCHENKO[3],

VIKTORIIA PODRYGA[3], PARVIN RAHIMLY[3]

[1] Damanhour University, E-mail: bakir.ae@phystech.edu

[2] Shirshov Institute of Oceanology of RAS, E-mail: gkazakevich@yandex.ru

[3] Keldysh Institute of Applied Mathematics of RAS, E-mail: hecon@mail.ru, pvictoria@list.ru, pervin@rehimli.info

The work considers numerical modeling of multiphase flow of liquids and gases in a porous medium with a nonlinear filtration law taking into account the dissociation of gas hydrates. Modeling is based on the support operator method [1]. This method allows discretization of partial differential equations on irregular grids, which makes it possible to approximate processes in layers of complex geological and geometric structure. The application of these methods to study gas release from the earth's interior during the decomposition of gas hydrates is considered.

Currently, in connection with climate threats, the world pays increased attention to the problem of greenhouse gas emissions from the earth's interior. The scale of such emissions (methane seeps) is especially large on the ocean floor, their traces on the bottom are many local ring structures of the funnel type (pockmarks), under them extended vertical structures have been discovered, indicating an influx of gas from the lower horizons. A detailed review for 2007 is given in the monograph [2]. Since then, many new pockmarks have been found. Similar structures are also formed on land, in particular, in the permafrost zone. The reason for the intensive vertical migration of gas

is considered to be the occurrence of a high-pressure region in the earth's interior, from where a gas breakthrough occurs, which can be explosive in nature with a sharp ejection of rock and the formation of a funnel, or less intense, leading to the occurrence of highly permeable channels in the reservoir systems, through which gas is carried upward. The mechanisms of formation of such channels are studied theoretically and experimentally [3, 4].

One of the possible causes of abnormally high pressures in formations may be the decomposition of underground gas hydrate deposits, resulting in the release of approximately 160 volumes of gas per volume of hydrate. The causes of hydrate decomposition are increased temperature, seismic disturbances, etc. Metastable gas hydrates located at shallow depths in permafrost zones are especially sensitive. Since gas hydrates contain huge reserves of methane, then, as shown in a significant number of works, starting with [5], its release may have a significant impact on the climate.

The physical basis is the equations of mechanics of saturated porous media, based on the laws of conservation of mass and energy and taking into account the complex thermodynamics of a multiphase multicomponent medium filling the pore space and containing solid gas hydrate inclusions. Usually, the linear filtration law (Darcy's law) is used for such problems. But since vertical gas migration through highly permeable channels can occur at a high speed, calculations are based on the quadratic Forchheimer law [6].

The advantage of the approach based on the support operator method is the automatic transfer of conservation laws that are satisfied for a continuous model to the discrete case. This is achieved by mutually consistent approximation of vector analysis operations - divergence and gradient, which allows the inclusion of all possible

modifications of the flow laws between different grid cells in the system, including the nonlinear filtration law.

Two models of a gas hydrate reservoir subjected to thermal action are considered as typical problems. The first model, which allows approximation on a regular grid, considers gas release during heating of a thin horizontal gas hydrate reservoir located between layers of impermeable rocks. It is assumed that when the pressure is high, but insufficient for explosive destruction of the rock, a crack begins to develop in some place, growing under the influence of gas breaking through into it. The mechanism of crack development is not studied here, it is introduced as a vertical channel of increased conductivity through which the gas comes out. The second model considers a gas hydrate reservoir of more complex geometry, convex upward. Here, an irregular grid is used for approximation. Since the gas begins to concentrate in the upper part of the reservoir (lithological trap), the breakthrough occurs there. The efficiency of the support operator method for calculating such breakthroughs in problems without hydrates was previously shown in [7]. A brief review of works on the influence of deformations of overlying layers on gas breakthrough is given in [4].

Keywords: gas hydrate dissociation, numerical modeling, nonlinear filtration, support operator method, multiphase flow, irregular grids, pockmarks, methane seeps

References:

[1] A. A. Samarskii, A. V. Koldoba, Yu. A. Poveshchenko, V. F. Tishkin, A. P. Favorskii. 1996. Difference schemes on irregular grids. ZAO «Kriteriy», Minsk. 273 p. (in Russian)

[2] A. Judd, M. Hovland. 2007. Seabed fluid flow: the impact on geology, biology and the marine environment. Cambridge University Press, Cambridge, U. K. 475 p. doi: 10.1017/CBO9780511535918.

[3] L. Räss, N. S. Simon, Y. Y. Podladchikov. 2018. Spontaneous formation of fluid escape pipes from subsurface reservoirs. Scientific reports. Vol. 8, No. 1, pp. 1-11. doi:10.1038/s41598-018-29485-5

[4] I. Vaknin, E. Aharonov, R. Holtzman, O. Katz. 2024. Gas seepage and pockmark formation from subsurface reservoirs: insights from table- top experiments. Journal of geophysical research: solid earth. Vol. 129, Paper e2023JB028255. doi:10.1029/2023JB028255.

[5] J. P. Kennett, K. G. Cannariato, I. L. Hendy, R. J. Behl. 2003. Methane hydrates in quaternary climate change: the clathrate gun hypothesis. American Geophysical Union,

Washington DC. 217 p. doi:10.1029/054SP

[6] R. E. Collins. 1961. Flow of fluids through porous materials. Reinhold Publishing Corp., New York. 270 p.

[7] G. I. Kazakevich, E. A. Minervina, Yu. A. Poveshchenko. 2002. Hydrocarbon migration in the process of pool formation: numerical modeling of nonlinear effects. Doklady Earth Sciences. Vol. 383, No. 2, pp. 198-200.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

A Kriging-assisted first order reliability method combining heuristic algorithms for efficient and accurate reliability analysis

Shiyuan Yang [1,a], Abílio M.P. De Jesus [2], Debiao Meng [3], Shun-Peng Zhu [4]

[1] University of Porto, E-mail: up202311575@edu.fe.up.pt

[2] University of Porto, E-mail: ajesus@fe.up.pt

[3] University of Electronic Science and Technology of China, E-mail: dbmeng@uestc.edu.cn

[4] University of Electronic Science and Technology of China, E-mail: zspeng2007@uestc.edu.cn

Efficient and accurate structural reliability analysis is a crucial challenge for complex structural reliability analysis problems including low failure probabilities [1, 2]. The classical First-Order Reliability Method (FORM), due to the ever-increasing nonlinear of the Limit State Function (LSF), may lead to higher and higher calculation errors. In this work, a Kriging Model-assisted FORM combining Heuristic Algorithms Framework (KM-HAF) is proposed to enhance the performance of reliability analysis for FORM. In particular, an enhanced constraint handling method based on an augmented lagrangian penalty function is developed to improve the computational accuracy of FORM based on a heuristic algorithm. An efficient Kriging model-building strategy combined with FORM and corresponding stopping criteria is applied for training the Kriging model which is utilized for efficient reliability analysis. Using four numerical and three engineering problems, the Kriging model-assisted structural reliability analysis frameworks coupling FORM with the heuristic algorithm are compared to the classical FORM algorithm, popular FORM-based on a heuristic algorithm and Kriging-based

sampling methods. The results show that KM-HAF has greater advantages in the number of calling LSF, computational accuracy, and robustness.

Keywords: First-order reliability method; Kriging model; Heuristic algorithm; Augmented lagrangian penalty function

---

[a] Presenting Author

References:

[1] T. Zhou, X. Zhu, T. Guo, Y Dong, M. Beer. 2025. Multi-point Bayesian active learning reliability analysis. Structural Safety. Vol. 114, pp. 102557.

[2] A. Savvides, M. Papadrakakis. 2022. Uncertainty quantification of failure of shallow foundation on clayey soils with a modified cam-clay yield criterion and stochastic fem. Geotechnics. Vol. 2(2), pp. 348-384.

s

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Influence of Computational Cell Aspect Ratio on the Accuracy and Computational Cost of CFD Simulations of Gas-Accelerated Flat Sheet Jets

Krištof Kovačič [1,a], Božidar Šarler[1,2]

[1] Faculty of Mechanical Engineering, University of Ljubljana, Slovenia, E-mail: kristof.kovacic@fs.uni-lj.si

[2] Institute of Metals and Technology, Ljubljana, Slovenia E-mail: bozidar.sarler@fs.uni-lj.si

This study examines the impact of computational cell aspect ratio on the accuracy and computational cost of Computational Fluid Dynamics (CFD) simulations of gas-accelerated flat sheet jets, also known as liquid sheets. The computational model, based on the Finite Volume Method (FVM), simulates unsteady, laminar, two-phase flow, treating gas as compressible and water as incompressible. The Volume of Fluid (VOF) method with piecewise linear interface calculation (PLIC) ensures precise gas-liquid interface tracking, while Adaptive Mesh Refinement (AMR) reduces the computational cost. Meshes with aspect ratios greater than one are compared against a reference simulation using a uniform mesh, experimentally validated with a 6% error, to evaluate the trade-off between accuracy and computational efficiency. The analysed case is characterised by a gas Reynolds number of 351, a liquid Reynolds number of 332, a Weber number of 51, and a Capillary number of 0.15 and is performed in atmospheric conditions. This study establishes a basis for determining the optimal combination of mesh aspect ratio that minimises computational cost while preserving accuracy, which is essential for future simulations of sheet jets under vacuum conditions. In such environments, where the sheet thickness is two orders of magnitude smaller, computational costs rise significantly, making efficient meshing strategies crucial for enabling high-fidelity simulations within practical timeframes.

Keywords: Gas-accelerated flat sheet jet, liquid sheet, CFD, VOF, cell aspect ratio

[a] Presenting Author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Multiscale Automated Discovery Approach for Homogenized Material Identification in Metamaterials

Mohammad Shojaee[1,a], Oliver Weeger[1]

[1] Cyber-Physical Simulation, Department of Mechanical Engineering, TU Darmstadt, Germany, E-mail: shojaee@cps.tu-darmstadt.de

This study presents an automated method for identifying the homogenized material properties of metamaterials. Through a framework based on first-order homogenization theory, an automated material discovery approach is proposed to determine these properties. The methodology employs physics-based constraints to derive hyperelastic constitutive laws for cubic symmetry metamaterials. Boundary stress data and displacement fields obtained from full-scale simulations in Abaqus serve as input, ensuring realistic and applicable results. Additionally, this information can be obtained experimentally. By enforcing equilibrium constraints both within the bulk and at loaded boundaries, the proposed approach generates interpretable and sparse models through *lp*-regularized regression and nonlinear optimization [1]. The effectiveness of the discovered models is validated by comparing the homogenized material properties with micromechanical models, demonstrating strong agreement. Notably, while micromechanical models have limitations in capturing different strain energy models, the proposed framework is general and adaptable. Furthermore, this approach extends to generalized continuum theories, such as micromorphic theory, enhancing its applicability [2].

The methodology integrates full-scale simulations from Abaqus with isogeometric analysis (IGA) to interpolate displacement fields and compute the homogenized deformation gradient. Various loading conditions, including simple shear, pure shear, biaxial, uniaxial, and pure bending, are considered to assess the homogenized material

behavior. The first Piola- Kirchhoff stress tensor is derived from the strain energy function as a function of material parameters. Internal nodal forces and reaction stresses at the boundary are analyzed to ensure linear momentum balance. The study demonstrates that first-order homogenization effectively captures the mechanical response of metamaterials, making it a valuable tool for advanced material design and optimization. This framework is particularly beneficial for characterizing the homogenized behavior of metamaterials, enabling efficient and accurate property identification for advanced engineering applications.

Keywords: Multiscale modeling, Automated Discovery Approach, Metamaterials, Material Identification

---

[a] Presenting Author

References:

[1] M. Flaschel, S. Kumar, L. De Lorenzis. 2021. Unsupervised discovery of interpretable hyperelastic constitutive laws. Computer Methods in Applied Mechanics and Engineering. Vol. 381, p. 113852.

[2] Shojaee, M., Mohammadi, H., & Weeger, O. 2024. Nonlinear micromorphic Timoshenko beam modeling and vibration analysis of microstructured beams. In International Journal of Non-Linear Mechanics. Vol. 166, p. 104861.

Numerical Investigation on Convective Heat Transfer Enhancement by Ionic Wind

Pejman Naderi, Dominic Groulx, Alex Martynenko[a]

Dalhousie University, NS, Canada. E-mail: alex.martynenko@dal.ca

An innovative heat transfer enhancement approach involves the application of an electric field to facilitate forced convection flow at the gas-material interface. In this method, a high-voltage electric discharge ionizes the air near a discharge electrode, and the movement of these ions toward a grounded electrode generates a flow of air known as ionic wind [1]. When combined with crossflow, this ionic wind enhances heat and mass transfer, a concept that has been experimentally verified [2]. Numerical simulations have also been conducted on a multi- pin discharge electrode to explore the limits of crossflow speed and the interaction between these two types of fluid [3]. However, scaling up electrohydrodynamic (EHD) drying for industrial applications presents certain challenges. Using pins as discharge electrodes may not be practical on a larger scale. In contrast, using wires as discharge electrodes offers the advantage of easier setup and replacement.

The schematic of the computational domain is shown in Fig. 1. Cross-airflow enters the channel from the left. The lower plate is electrically grounded. A 25 cm-long section, located 50 cm downstream from the inlet, is selected for heat exchange within the 2D domain. This plate transfers heat to the moving air, and the heat transfer coefficient will be analyzed. The discharge electrode is modelled as a circle (wire) with a radius of 0.2 mm, positioned 4 cm above the grounded electrode inside the channel. The wire is supplied with a high-voltage DC source. The airflow is assumed to be incompressible, and its initial temperature is 21°C.

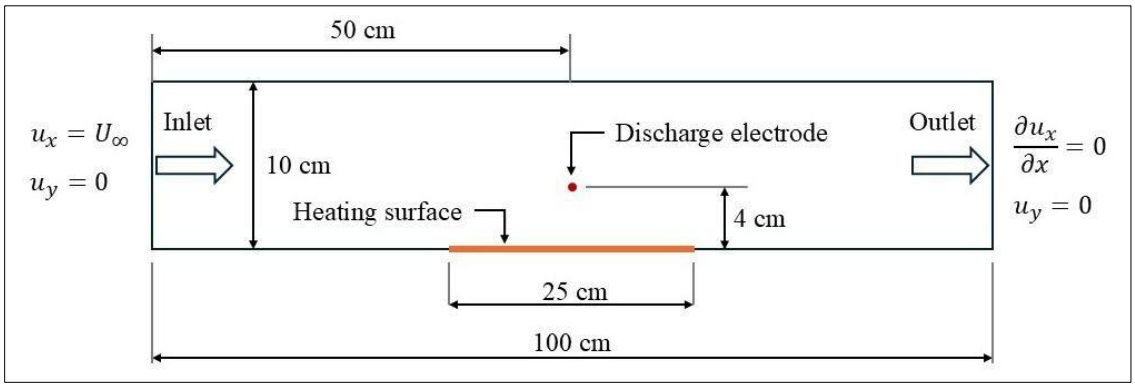


Figure 1. Schematic diagram of the computational domain.

The recent COMSOL 6.3 version contains an Electric Discharge module, which allows the simulation of the electric discharge effect on heat and mass transfer. COMSOL simulations of coupled electric discharge and laminar flow simultaneously solved electric field and fluid dynamics. Poisson's equation was used to calculate the electric potential, based on electrode voltages and the space charge density, which determines the electric field. Charge transport

[a] Presenting Author

equations, including drift, diffusion, and reactions (ionization, recombination), update the space charge density, which in turn influences the electric field. The laminar fluid flow module solves the Navier-Stokes equations, where the electric body force (space charge density times the electric field) acts as a source of momentum, affecting the airflow. This creates a feedback loop, with the electric field influencing the flow and the flow affecting the charge transport. COMSOL iteratively solves these coupled equations until a converged solution is achieved.

The preliminary result is presented in Fig. 2, where the inlet velocity is 1 m/s, and the high-voltage wire is charged at 27 kV. The ionic wind contributes to accelerating the crossflow and reducing the thickness of the boundary layer near the grounded electrode. This reduction increases the temperature gradient at the surface, enhancing heat transfer. Further investigation could focus on optimizing the ratio of EHD flow to crossflow for maximum heat transfer. Additionally, the orientation of the wire, the gap between the wire and counter electrode, the wire diameter, and multiple wire arrangements can also be explored through simulation.

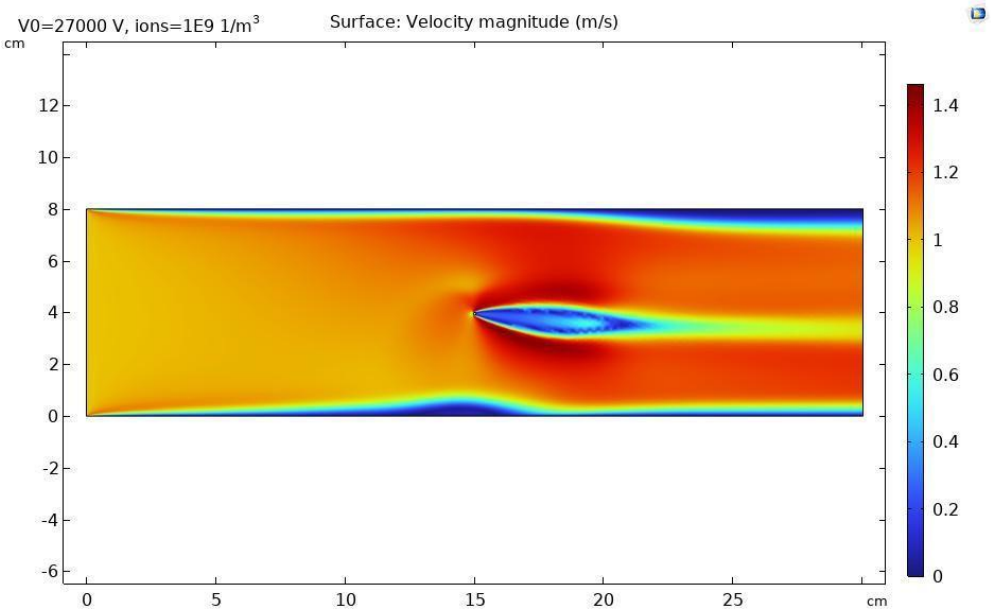


Figure 2. Boundary layer distortion influenced by EHD flow.

Keywords: Electrohydrodynamic (EHD) drying, Ionic wind, Heat and mass transfer, Forced convection

References:

[1] M. Rickard, D. Dunn-Rankin, F. Weinberg, F. Carleton. 2005. Characterization of ionic wind velocity. Journal of Electrostatics, Vol 63, pp. 711–716.

[2] M. Hamdi, O. Rouaud, D. Tarlet, M. Havet. 2021. Experimental investigation on convective heat transfer enhancement by EHD in wire-to-plate configuration. Journal of Thermal Science and Engineering Progress, Vol 26, pp. 101086.

[3] C. Zhong, A. Martynenko, P. Wells, K. Adamiak. 2019. Numerical investigation of the multi-pin electrohydrodynamic dryer: Effect of cross-flow air stream. Journal of Drying Technology, Vol 37, pp. 1665–1677.

Multiscale Calculations of Metal Coating Spraying Processes

PODRYGA V. O. [1,a], POLYAKOV S. V. [2], TARASOV N. I. [3]

[1] Keldysh Institute of Applied Mathematics of RAS, E-mail: pvictoria@list.ru

[2] Keldysh Institute of Applied Mathematics of RAS, E-mail: polyakov@imamod.ru

[3] Keldysh Institute of Applied Mathematics of RAS, E-mail: nikita_tarasov@imamod.ru

The study of spraying processes has traditionally been an important component of nanotechnology improvement. At the present stage, there has been a qualitative leap in the field of miniaturization of microelectronic components, medical devices, and active biological objects manufactured using various spraying methods. However, the obstacle to their widespread implementation is the low quality of the final products and their high cost. To overcome this difficulty, a comprehensive theoretical analysis of existing spraying technologies is required, taking into account the multiscale nature of the process and relying on mass computer calculations.

In the work, the technology of supersonic cold gas-dynamic spraying (SCGDS) [1, 2] the metal nanoclusters on substrates is studied. It is used to create ultra-thin coatings for micro- and nanoelectronics. The advantage of SCGDS is its relative cost-effectiveness and controllability. To analyze the spraying processes within the framework of SCGDS, the authors developed earlier a two- scale approach [3, 4], based on a combination of macroscopic and microscopic models. A quasi- gasdynamic system of equations [5] in a three-dimensional formulation, supplemented by convection- diffusion equations for the concentration of sprayed metal nanoparticles, is used as a macroscopic model. The equations of classical molecular dynamics [6] are used as a microscopic model. The macroscopic model is implemented using the finite volume grid method [7]. The microscopic model is implemented using the velocity

Verlet integration [8]. The conjugation of the models is performed using statistical physics methods.

In this work, in addition to the above-described two-scale computational technology, a three- scale modification of the approach has been developed that includes a mesoscopic level. The description of processes at the mesoscopic level is based on the application of the modified smoothed particle hydrodynamics [9] and is aimed at a detailed consideration of the transition between macroscopic and microscopic processes. For this version of the three-scale model, a comprehensive numerical technique and a parallel program oriented towards supercomputer calculations were created. Using the developed program tools, a series of numerical calculations of nickel and copper nanoparticles spraying on substrates were performed. They confirmed the correctness of the developed multiscale approach, the efficiency of the proposed computer implementation and the possibility of its use in planning full-scale experiments.

Keywords: supersonic cold gas-dynamic spraying, multiscale mathematical model, combination of finite volume grid method and particle methods, supercomputer calculations.

References:

[1] A. Papyrin, V. Kosarev, S. Klinkov, A. Alkhimov, V. Fomin. 2007. Cold spray technology. Elsevier Science, Amsterdam.

[2] P. Poza, M.A. Garrido-Maneiro. 2022. Cold-sprayed coatings: microstructure, mechanical properties, and wear behavior. Prog. Mater. Sci. Vol. 123, Paper 100839.

[3] V.O. Podryga, S.V. Polyakov, N.I. Tarasov, V.A. Usachev. 2023. Mathematical modeling the processes of supersonic cold gas dynamic spraying of nanoparticles on substrates. Lobachevskii Journal of Mathematics. Vol. 44, No. 5, pp. 1918-1928.

[4] V.O. Podryga, S.V. Polyakov, G.A. Bagdasarov, P.I. Rahimly. Two-scale modeling of supersonic cold gas dynamic spraying of nanoparticles on substrate. AIP Conference Proceedings.

[a] Presenting Author

2024. Vol. 3094, No. 1, Paper 500025.

[5] T.G. Elizarova. 2009.Quasi-gas dynamic equations. Springer-Verlag, Berlin, Heidelberg.

[6] D.C. Rapaport. 2004. The art of molecular dynamics simulation. Cambridge Univ. Press, Cambridge.

[7] R. Eymard, T. R. Gallouet, R. Herbin. 2000. The finite volume method. In: Handbook of Numerical Analysis. North-Holland, Amsterdam, Vol. 7, pp. 713-1020.

[8] L. Verlet. 1967. Computer "experiments" on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules. Phys. Rev. Vol. 159, pp. 98-103.

[9] J.J. Monaghan. Smoothed particle hydrodynamics and its diverse applications. 2012. Annu. Rev. Fluid Mech. Vol. 44, pp. 323-346.

Construction of Topological Spherical Quadrilateral Meshes Based on Meromorphic Differentials

Hao Wang1, Xiaopeng Zheng2,*, Jun Yue3,Na Lei4,Zhongxuan Luo5 [1]Dalian University of Technology, E-mail: wanghao@mail.dlut.edu.cn

[2]Dalian University of Technology, E-mail: zhengxp@dlut.edu.cn [3]Dalian University of Technology, E-mail: junyue0420@163.com [4]Dalian University of Technology, E-mail: nalei@dlut.edu.cn [5]Dalian University of Technology, E-mail: zxluo@dlut.edu.cn

Abstract: In recent years, the rapid advancement of computational devices has imposed increasingly strin- gent requirements on finite element mesh generation for practical numerical simulations. Among surface meshes, semi-structured quadrilateral meshes exhibit superior computational performance in certain do- mains compared to triangular meshes. The equivalence between quadrilateral meshes and meromorphic quartic differentials has recently been rigorously established through mathematical theory. This paper pro- poses a method for constructing topological spherical quadrilateral meshes based on meromorphic quartic differentials.

This paper connects the topological spherical model to meromorphic differentials via stereographic projection and spherical harmonic mapping, enabling the generation of quadrilateral meshes for the topological spherical model. First, a quasi-conformal mapping between the topological spherical model and the unit sphere is constructed

using spherical harmonic mapping, preserving the original curvature information of the model. Subsequently, the zero and pole locations of the meromorphic function on the complex plane are determined based on the model's curvature information, and the meromorphic function is constructed to generate the quadrilateral mesh. Finally, the planar quadrilateral mesh is mapped back to the original model through inverse mapping, yielding the quadrilateral mesh of the topological spherical model.

This paper proposes a universal, controllable, and theoretically guaranteed method for generating topological spherical quadrilateral meshes. Experimental results validate the effectiveness of the proposed approach. The main contributions of this paper are as follows:

- Universality: By utilizing stereographic projection and spherical harmonic mapping, a mapping is established between meromorphic differentials on the complex plane and topological spherical models.
- Controllability: By integrating the curvature information of the original surface, the positions of zeros and poles on the complex plane are determined, thereby controlling the locations of singular points in the quadrilateral mesh.
- Robustness: This method is theoretically rigorous.

Keywords: Quadrilateral Meshes, Meromorphic Differential, Topological Sphere

* Presenting author

References

[1] Wei Chen, Xiaopeng Zheng, et al. 2019. Quadrilateral mesh generation I : Metric based method. Computer Methods in Applied Mechanics and Engineering. Vol. 356, pp. 652- 668.

[2] XiaoPeng Zheng, Yiming Zhu, et al. 2021. Quadrilateral mesh generation III : Optimizing singularity configuration based on Abel–Jacobi theory. Computer Methods in Applied Mechanics and Engineering. Vol. 387, pp. 114-146.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

A Numerical Method for Solving Maxwell's Equations in Singular 3D Geometry

Franck Assous [1], Irina Raichik[2,*]

[1]Ariel University, E-mail: assous@ariel.ac.il

[2]Bar-Ilan University, E-mail: irina.raichik@gmail.com

Abstract: We propose a variational method to compute the three-dimensional Maxwell equations in an axisymmetric singular domain generated by the rotation of a singular polygon around one of its sides, which contains reentrant corner or edges. Due to the axisymmetric assumption, the singular computational domain reduces to a subset of R^2. However, the electromagnetic field and other vector quantities still belong to R^3.

Taking advantage of the fact that the domain becomes two-dimensional, through Fourier analysis in the third dimension, one arrives to a sequence of singular problems set in a 2D domain, depending on the Fourier variable *k*. Under these conditions, the 3D solution is solved by addressing several 2D problems, each de- pendent on *k*.

Furthermore, for each mode *k*, we can show that the solution can be decomposed into a regular and a singular part. Therefore, the regular part can be computed using a classical finite element method. The singular part belongs to a finite-dimensional subspace, its dimension being equal to the number of reentrant corners and edges of the 2D polygon that generates the 3D domain.

We first compute this singular part using an *ad hoc* numerical method only for $k = 0, \pm 1, 2$, where the mode $k = 2$ appearing as a "stabilization" mode for all other *k*. Then, the total solution will be computed based on a non-stationary variational formulation. Numerical examples will be presented to illustrate that the proposed method can capture the singular part of the solution. This approach can also be viewed as the generalization of the Singular Complement Method to time-dependent three-dimensional axisymmetric problem [1], [2].

Keywords: Time-dependent Maxwell equations, Fourier analysis, Singularities, Axisymmetric geometry

---

* Presenting author

References

[1] F. Assous, I. Raichik, Numerical solution to the 3D static Maxwell equations in axisymmetric singular domains with Arbitrary Data, *J. Comput. Meths. Appl. Maths*, 20-3, 419-435 (2020).

[2] F. Assous, P. Ciarlet, Jr., and S. Labrunie *Mathematical Foundations of Computational Electromagnetism* Appl. Math. Sc., AMS 198, Springer (2018).

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P

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

Integrating Multi-Scale and Multi-Uncertainty Analysis in Structural Reliability Assessment

TEMPLE NJOKU [1],**a**, **CHENFENG LI** [2]

[1] Swansea University, E-mail: 234l677@swansea.ac.uk

[2] Swansea University, E-mail: c.f.li@swansea.ac.uk

In high-risk settings such as offshore platfonns, bridges, and tall buildings, structural reliability assessment is essential in ensuring the durability and safety of engineering infrastructure. However, the conventional techniques of structural reliability analysis often fail to fully account for the multi-scale interactions and uncertainty propagation across structural levels, which impacts on the accuracy of the estimated reliability indices. To enhance the accuracy of structural reliability estimates, this paper proposes a computational framework that combines multi-scale modelling with multi-uncertainty quantification.

The proposed approach employs computational homogenization methods to convert material-level uncertainties (e.g., variability in mechanical characteristics, corrosion progression) into system-level reliability evaluations. The degradation mechanisms, environmental variables, and loading condition uncertainties are all considered using stochastic finite element modelling (SFEM). In addition, real-time updating ofreliability estimates based on inspection data is made possible via Bayesian inference and surrogate models based on Gaussian processes. Monte Carlo simulation and Importance Sampling approaches are further integrated into the framework to calculate low-probability failure occurrences effectively.

This paper focuses only on the theoretical formulation and computational methods of a system intended to evaluate inspection data from a fixed offshore platform. The validation method will be examined in future research. The results enhance risk-informed decision-making by offering a scalable and computationally efficient method for improving structural engineering inspection planning and maintenance methods.

---

[1] Presenting Author

References:

[1] Tang, Y.; Zhang, X.; Gu, H.; Li, K.; Hong, C.; Tu, S.; Sato, Y., Wang, R. 2025. Structural reliability assessment under creep-fatigue considering multiple uncertainty sources based on surrogate modeling approach. *International Journal of Fatigue.* Vol. 192, 108728.

[2] Zhou, H.; Li, J.; Ren, X. 2016. Multiscale stochastic structural analysis toward reliability assessment for large complex reinforced concrete structure, *International Journal for Multiscale Computational Engineering,* Vol 14(3), pp 303-321.

[3] Zhou, X.; Wang, N.; Xiong, W.; Wu, W.; Cai, C. 2022. Multi-scale reliability analysis of **FRP** truss bridges with hybrid random interval uncertainties, *Composite Structures,* Vol 297 115928.

[4] Shahraki, A. F.; Yadav, 0. P.; Liao, **H.** 2017. A review on degradation modeling and its engineering applications, International Journal of Performability Engineering, Vol 13 (3), pp 299-314

This work seeks to bridge the gap between structural-scale risk assessment and material-level variability, advancing the area of multi-scale reliability analysis. It also offers a robust approach for academics and engineers seeking to improve structural integrity estimations in the face of uncertainty.

Keywords: multi-scale modelling, structural reliability, uncertainty quantification, Bayesian inference, stochastic finite element modelling, probabilistic risk assessment.

Image-Based simulation of porous insulation materials

Liam Jaarsveld Garcia[1]

[1] 852953@swansea.ac.uk

The application of new insulation materials within the industry that look to increase safety, efficiency and resilience traditionally requires accelerated testing to ensure compliance with safety standards and regulation. These tests will typically require substantial expense and time to conduct, impacting innovation. This research will perform image-based computational simulations of heat conduction and convection in heterogeneous and porous insulation materials.

First, images of insulation materials are taken using the ZEISS Xradia 520 Versa XRM

[1] to analyze their microstructural features. The acquired images are segmented and reconstructed to reduce noise and generate a high-fidelity mesh that accurately represents the porous structure. Finally, a multi-physics simulation is conducted in OpenFOAM [2] to model heat conduction and convection within the solid matrix and fluid domains.

This study aims to provide a cost-effective and efficient alternative to traditional experimental testing for insulation materials by leveraging image-based computational modeling. The insights gained from these simulations predicting the material's thermal performance can help limit the number of materials in which physical testing is performed, reducing the time and cost of developing the next generation of insulation materials.

Keywords:

- Porous media

- Image-Based Simulation
- Multi-physics Simulation
- Computational modelling
- Thermal Performance
- Heat Transfer
- X-ray Microscopy

References:

[1] ZEISS Xradia Versa User's Guide [Internet]. 2016 [cited 2025 Mar 2]. Available from: https://www.physics.purdue.edu/xrm/new-users/training/Xradia_Versa_Users_Guide_v11x_510.pdf

[2] H. G. Weller, G. Tabor, H. Jasak, C. Fureby, A tensorial approach to computational continuum mechanics using object-oriented techniques, COMPUTERS IN PHYSICS, VOL. 12, NO. 6, NOV/DEC 199

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Image-based Microstructural Simulations of polycrystalline Materials

Bingbing Chen[1,*], Chengfeng Li[2]

[1]Swansea University, E-mail: Bingbing.chen@swansea.ac.uk

[2]Swansea University, E-mail: c.f.li@swansea.ac.uk

Abstract: Polycrystalline materials, including metals, rocks, and ceramics, are prevalent in nature and industry. Their formation involves nucleation and growth via solidification, recrystallisation, grain growth, and solid-state phase transformation. These complex evolution processes lead to polycrystalline microstruc- tures with random crystallographic and morphological features, comprising grain aggregates with varying lattice orientations, sizes, and shapes, separated by grain boundaries. Random characteristics of polycrys- talline microstructures significantly influence the macroscopic properties and performance of polycrystalline materials. In recent years, extensive correlation studies have been conducted between microstructure char- acterisations and macroscopic properties and performance in polycrystalline materials. These studies have demonstrated that microstructural variability within polycrystalline materials substantially impacts their macroscopic performance. In particular, features such as grain size, crystallographic orientation, and grain boundary are pivotal in governing the overall mechanical and physical properties of polycrystalline materials.

However, in current practice, studies of the microstructure effect on mechanical properties and performance have certain limitations. For example, the research methodologies are primarily limited to representative volume element (RVE)-based experimental reconstruction. In practice, the microstructure characterisations exhibit some degree of randomness during deformation processing, and microstructure randomness reveals polycrystalline materials' probabilistic properties and performance. Consequently, the vast size and number of the microstructure RVE necessary to build the structure–properties linkages are computationally pro- hibitive and challenging to investigate. Meanwhile, the simplified polycrystalline microstructures, such as single crystals, bicrystals, Voronoi, and ellipsoid polycrystals, fail to capture all the statistical microstructure characterisations of the heterogeneous grains. Furthermore, to the author's knowledge, these features that influence mechanical properties and performance are still contentious, and the association between them is not yet wholly researched. In addition, it is difficult to quantify the impact of microstructure on mechanical properties and performance in polycrystalline materials without a straightforward and efficient method. Ul- timately, the datasets between microstructural characteristics and mechanical properties and performance are unlikely to be built without sufficient data.

This research first investigates the recent progress in the digital reconstruction of polycrystalline materials. After that, a novel data-driven digital reconstruction method for polycrystalline microstructures is proposed to enable efficient reconstructions with high fidelity to actual microstructural characteristics. Moreover, combined with feature-specified and constraint-controlled reconstruction algorithms, the established crystal plasticity model is employed to perform a quantitative analysis of polycrystalline materials, fully under- standing the macroscopic properties and performance responses concerning random microstructural features. Finally, structure-property datasets are built by coupling

crystal plasticity finite element simulation and the data-driven feature-specified and constraint-controlled reconstruction algorithms. These datasets show excel- lent potential in optimising manufacturing processes (cause-effect design) or developing new polycrystalline materials (goal-driven design).

Keywords: Alloy material,Microstructural reconstruction, Crystal plasticity finite element, Representative volume element, Structure-property linkage, Electron backscatter diffraction

---

* Presenting author

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Enhancement of a Crane Hook Design using Topology Optimization and AI-Based Generative Design for Weight Reduction

Eren KALAY [1,a], Adem CANDAS [2], C. Erdem IMRAK [3]

[1] Faculty of Mechanical Engineering, Istanbul Technical University, E-mail:kalaye@itu.edu.tr

[2] Faculty of Mechanical Engineering, Istanbul Technical University, E-mail:candas@itu.edu.tr

[3] Faculty of Mechanical Engineering, Istanbul Technical University, E-mail:imrak@itu.edu.tr

In the previous decade, the implementation of topology optimization and generative design has gained significant momentum in structural and mechanical engineering [1,2], particularly in load-bearing systems. This growth has been driven by the increasing accessibility of computational power and additive manufacturing capabilities. These advanced computational approaches enable the development of innovative and optimized design solutions that balance efficiency and manufacturability by integrating physics simulations with optimization algorithms. This work explores the application of topology optimization and generative design methodologies in the design of high-performance crane hooks, overcoming the drawbacks of classical empirical design and stress analysis techniques, which frequently lead to overweight structures

with unnecessary material consumption. Advanced optimization techniques enable structures to achieve significant weight reduction while enhancing strength and fatigue resistance. Topology optimization effectively removes redundant material while generative design utilizes AI-driven algorithms to identify innovative yet structurally practical configurations.

Recently, Finite Element Method (FEM) was used to evaluate the crane hook's numerical model before applying the optimization method to assess its structural integrity certain under loading conditions [3]. A validation test was conducted using an experimental tensile test on a crane hook, confirming that the initial numerical predictions accurately reflected its real mechanical behavior [4]. A commercial 3D modeling software was used to optimize the design of a hook, ensuring both sufficient strength and weight reduction [5]. Validating the reliability of the pre-optimized model further strengthened confidence in the optimized crane hook design. This study evaluates the feasibility of integrating topology optimization and generative design in crane hook design focusing weight reduction while maintaining structural reliability. The key factors examined include stress distribution, deformation characteristics under tensile loading conditions, manufacturability, and computational efficiency. This study aims to develop high-performance crane hook designs that achieve significant material savings while maintaining structural integrity and manufacturability, using modern

[a] Presenting Author

computational methods such as Finite Element Analysis (FEA) and AI-driven optimization techniques.

This study illustrates the effectiveness of applying topology optimization and generative design in creating high-performance crane hooks given in the TS-ISO 15401 standard. Finite Element Analysis (FEA) was employed to examine the structural integrity of the crane hook under vertical loads, both before to and during optimization of the designs. The findings validate that both topology optimization and generative design provide significant weight reduction while maintaining sufficient strength. Topology optimization decreased the crane hook's weight by 14.4% while maintaining stress levels within the acceptable range. Despite the weight decrease, the Maximum principal stress remained within permissible limits, rising from 224.85 MPa in the original design to 290.98 MPa in the improved model, which remains below the material's yield strength. Generative design, alternatively, accomplished a notable weight reduction of 24%, but at the cost of more intricate geometries necessitating advanced manufacturing techniques. However, the maximum principal stress reached

298.12 MPa, which is still lower than yield strength and equivalent to the topology- optimized model. These findings show that, while topology optimization provides a well-balanced approach to weight reduction and manufacturability, generative design produces larger material savings by removing more non-load-bearing material, resulting in even lower weight. However, this comes at the cost of greater geometric complexity, making the production process more complicated and necessitating advanced manufacturing techniques. Future studies may focus on the experimental validation of the proposed optimized design.

Keywords: Generative design; Topology optimization; Crane hook; Finite element method; Tensile test

References:

[1] I.T. Teke, M. Akbulut, A.H. Ertas, Topology optimization and fatigue analysis of a lifting hook, Procedia Struct. Integr. 33 (2021) 75–83. https://doi.org/10.1016/j.prostr.2021.10.011.

[2] H. Kocabas, C.E. İmrak, Exact Analysis of Stresses in a Crane Hook, Tmt (2005). https://www.researchgate.net/publication/268923706.

[3] K. Kishore, V. Sanjay Gujre, S. Choudhary, A. Sanjay Gujre, M. Vishwakarma, T. Thirumurgan, M. Choudhury, M. Adhikary, A. Kumar, Failure analysis of a 24 T crane hook using multi-disciplinary approach, Eng. Fail. Anal. 115 (2020) 104666. https://doi.org/10.1016/j.engfailanal.2020.104666.

[4] S.A. Dhengle, Experimental Stress Analysis and Optimization of Crane Hook, (2020) 1451–1464.

[5] V.D. Hiep, N.X. Quynh, T.T. Tung, A topology optimization design of a crane hook (2024). Results Eng 23. https://doi.org/10.1016/j.rineng.2024.102492

Explicit Euler - Nonlocal Operator Method for Solving Transient Heat Conduction Problems

Umut Sahin [1,a]

[1] Istanbul Technical University, E-mail: sahinumu@itu.edu.tr

Numerical methods play a crucial role in solving transient heat conduction equations, which are central to numerous engineering applications. Traditional numerical approaches, including explicit and implicit finite difference methods (FDM), finite element methods (FEM), and finite volume methods (FVM), are widely utilized to tackle these equations. However, the choice among these methods typically hinges upon the complexity of the problem, desired computational efficiency, and accuracy requirements. While these methods are robust, they often lead to significant computational expense, especially when dealing with complex geometries or higher-dimensional spatial problems.

A higher order operator method is presented for boundary value problems by Ren et al. [1]. This study introduces a novel numerical approach by integrating a higher-order nonlocal operator method with the Euler explicit time-stepping scheme, denoted as EU-NOM. The proposed methodology effectively enhances computational efficiency and accuracy for solving higher-dimensional transient heat conduction problems. Unlike conventional local methods, the nonlocal nature of NOM provides an inherent capability to capture long-range spatial interactions, which can significantly improve solution fidelity.

The stability characteristics of the proposed EU-NOM scheme are rigorously analyzed, demonstrating that the method is conditionally stable. Comprehensive numerical simulations are conducted for both one-dimensional and two-

dimensional transient heat conduction scenarios, providing robust validation of the EU-NOM approach. Comparative analyses against established analytical solutions confirm that the EU-NOM method achieves high accuracy, validating its effectiveness and reliability.

Results show that the proposed method not only offers competitive accuracy but also significantly reduces computational overhead compared to traditional numerical methods. Therefore, the EU-NOM approach presents a promising alternative for efficiently solving transient heat conduction problems in engineering, particularly in scenarios demanding high computational precision and efficiency.

Keywords:

Nonlocal operator method; euler explicit method; transiet heat conduction problem

[a] Presenting Author

References:

[1] Ren, H., Zhuang, X., & Rabczuk, T. (2020). A higher order nonlocal operator method for solving partial differential equations. Computer Methods in Applied Mechanics and Engineering, 367, 113132.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
CM3P
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Deformation Mode Coupling and Size Effects in Micro-Architected Materials: Multi-Scale Modelling, Additive Manufacturing and Experimental Validation

Wanderson F. dos Santos[1], Alina S. L. Rodrigues[1], Igor A. Rodrigues Lopes[2,a], Francisco

M. Andrade Pires[2], Sergio P.B. Proença[1] and Zilda C. Silveira[1]

[1] Escola de Engenharia de São Carlos, Universidade de São Paulo, Av. Trabalhador São- Carlense, 13566-590 São Carlos, Brasil

[2] INEGI-LAETA, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 400, 4200-465 Porto, Portugal, ilopes@inegi.up.pt

Architected metamaterials may exhibit exotic mechanical behaviour, including deformation mode coupling (torsion-compression or shear-compression) and size effects. Some of these aspects are not captured by computational models based on classical continuum mechanics. Direct Numerical Simulations (DNS) of micro-architected structures are computationally demanding and multi-scale analyses based on FE2 approaches are an interesting alternative. However, classical first-order homogenisation may also fail to capture some deformation mechanisms since it is based on classical Cauchy continua. Therefore, a novel multi-scale second-order computational homogenisation formulation at finite strains [1], based on the Method of Multi-scale Virtual Power, is employed. The macro-scale is described by a second gradient theory, and the micro-scale Representative Volume Element (RVE) is modelled with the classical continuum theory, where the presence of a void phase is considered. The kinematics is

defined only in the solid domain of the RVE, where an appropriate expression is postulated for the homogenisation of the second-order gradient.

In this contribution, four types of lattice structures are analysed. First, a lattice promoting tension-compression coupling is assessed with both DNS and FE2 approaches. Since this coupling is due to higher-order mechanisms and size effects appear, it is only captured by FE2 based on second-order homogenisation. Second, a lattice based on N-shaped unit-cells, whose numerical models predict undulation induced by tension/compression [2], is 3D printed by Fused Deposition Modelling (FDM) and tested to obtain experimental data for validation of the numerical models. Plasticity is considered for this case, where it is shown that first-order homogenisation is adequate. Finally, triangular and square lattice structures manufactured using the same method are subjected to three-point bending. The experimental results show that size effects exist, and these can be captured by FE2 models with second-order homogenisation.

Keywords: Architected metamaterials, Deformation mode coupling, Additive manufacturing, Experimental validation, DNS models, FE2 multi-scale modelling

---

[a] Presenting Author

References:

[1] W.F. Dos Santos, et al. (2023). *Comput. Methods Appl. Mech. Eng.*, 416: 116374.

[2] W.F. Dos Santos, et al. (2024). *Int J Solids Struct.*;292:112724.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

A Comparative Review of Current Practices in Working Platform Design for Construction and Geotechnical Operations

Amir Arabzadeh [1,a], Chenfeng Li [2], Davide Deganello

[1] 2413570@swansea.ac.uk

[2] c.f.li@swansea.ac.uk

Working platforms are temporary geotechnical structures that are essential for providing stable support during operations, hence mitigating the risk of failure and overturning. Moreover, working platforms provide a weather-resistant operating surface with a minimum load-bearing capability, avoiding subgrade failure due to the movement of heavy machinery [1].

While foundation contractors primarily focus on piling rigs and other geotechnical equipment, everyone entering the site uses working platforms. Therefore, design considerations must also encompass cranes, concrete pumps, concrete trucks, delivery vehicles, and site staff [2]. A well-designed and correctly constructed working platform improves site efficiency, guarantees safety, and remains economical, benefiting all users. Proper platform design can achieve this objective. Multiple practical guides are available addressing the design, installation, maintenance, and repair of ground-supported working platforms for tracked plants, particularly BR470 and TWF 2019:02 being the most renowned. This study reviews and describes the primary design methods employed for working platforms, subsequently providing an overview of these methods.

Keywords: Working Platform, Temporary Works, Platform design, Geotechnical Structures

[a] Presenting Author

References:

[1] B. T. Chua, H. Abuel-Naga and K. P. Nepal. 2023. Design Charts for Geogrid-Reinforced Granular Working Platform for Heavy Tracked Plants over Clay Subgrade. Journal of Transportation Infrastructure Geotechnology. Vol. 10, pp. 795-815.

[2] The joint EFFC/DFI Working Platforms Task Group. 2019. Guide to Working Platforms. 1st Edition.

IACM SPECIAL INTEREST CONFERENCE
ECCOMAS Thematic Conference
COMPUTATIONAL METHODS FOR MULTI-SCALE, MULTI-UNCERTAINTY AND MULTI-PHYSICS PROBLEMS

Constitutive modeling of twinning induced deformation at elevated temperatures for MP35N superalloy

Ruijie-Deng[1,*], **Dongfeng-Li**[1]

[1]School of Science, Harbin Institute of Technology, Shenzhen 518055, China, E-mail: dengruijie@foxmail.com

[1]School of Science, Harbin Institute of Technology, Shenzhen 518055, China, E-mail:lidongfeng@hit.edu.cn

Abstract:

MP35N (35 wt% Ni–35 wt% Co–20 wt% Cr–10 wt% Mo) is a representative face-centred cubic (FCC) Ni–Co- based superalloy whose exceptional combination of ultrahigh yield strength, corrosion resistance and thermo- mechanical stability renders it indispensable for high-stress aerospace fasteners, high-temperature turbine components and down-hole drilling instrumentation. Under thermo-mechanical loading, plastic deformation in MP35N arises from the complex coupling of multiple physical processes, principally the dislocation slip mediated by dynamic strain aging (DSA) due to Cr and Mo solute drag and the nucleation-controlled tran- sition from stacking-fault accumulation to deformation twinning. These mechanisms interact dynamically across multiple scales and manifest macroscopically as serrated flow and reduced uniform elongation, both induced by the

intermittent pinning and unpinning of dislocations during DSA. At the mesoscale, heteroge- neous twinning causes strain redistribution that leads to surface roughening (the orange-peel effect) and the development of local necking instabilities.

To predict material behaviour under extreme conditions and optimise thermo-mechanical processing, we have developed a constitutive model that explicitly couples dislocation slip, twinning and DSA. Based on the thermally activated slip framework of Busso [1] and employing a Taylor homogenization scheme [2] to extend it to the macroscopic scale, the model accounts in detail for the contributions of the Hall–Petch effect [3], solute–dislocation interactions [4] and forest dislocation hardening [5] to overall slip resistance. Informed by the approach of Kalidindi [6], a pseudo-slip formulation with modified twinning geometry describes the nucleation kinetics of deformation twins, yielding a closed multi-mechanism constitutive framework.

Rigorous calibration of material parameters enables accurate capture of temperature-dependent serrated flow, yield strength degradation and strain-hardening behaviour. Simulated stress–strain responses show good agreement with the experimental data reported by Singh and Doherty [7]. Further analyses reveal that deformation twinning in MP35N exhibits pronounced temperature sensitivity, with twin nucleation occurring only at intermediate temperatures under quasi static uniaxial loading. Finally, finite-element simulations of a proportionally scaled specimen reproduce the propagation of Portevin–Le Chatelier (PLC) bands within a single stress-oscillation cycle and predict the spatiotemporal evolution of high-strain-rate bands along the specimen axis.

Keywords: MP35N superalloy, Constitutive model, Deformation twinning, Dynamic strain aging

---

* Presenting author

References

[1] Busso, E. P. (1998). A continuum theory for dynamic recrystallization with microstructure-related length scales. International Journal of Plasticity, 14(4-5), 319-353.

[2] Capolungo, L., Jochum, C., Cherkaoui, M., & Qu, J. (2005). Homogenization method for strength and inelastic behavior of nanocrystalline materials. International Journal of Plasticity, 21(1), 67-82.

[3] Hansen, N. (2004). Hall–Petch relation and boundary strengthening. Scripta Materialia, 51(8), 801-806.

[4] Wong, S. L., Madivala, M., Prahl, U., Roters, F., & Raabe, D. (2016). A crystal plas- ticity model for twinning-and transformation-induced plasticity. Acta Materialia, 118, 140-151.

[5] Taylor, G. I. (1934). The mechanism of plastic deformation of crystals. Part I.—Theoretical. Proceedings of the Royal Society of London. Series A, Containing Pa- pers of a Mathematical and Physical Character, 145(855), 362-387.

[6] Kalidindi, S. R. (2001). Modeling anisotropic strain hardening and deformation textures in low stacking fault energy fcc metals. International Journal of Plasticity, 17(6), 837- 860.

[7] Singh, R. P., & Doherty, R. D. (1992). Strengthening in multiphase (MP35N) alloy: Part II. elevated temperature tensile and creep deformation. Metallurgical Transactions A, 23, 321-334.