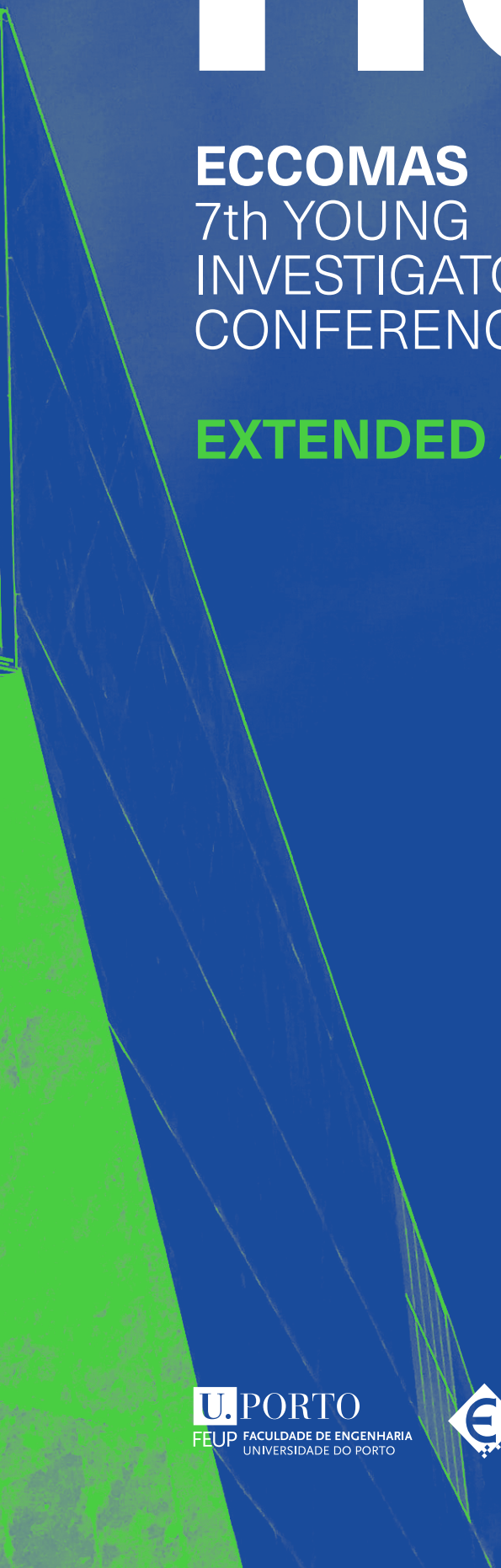
YIC23

ECCOMAS
7th YOUNG
INVESTIGATORS
CONFERENCE

FEUP
19—21
JUNE
2023

EXTENDED ABSTRACTS



U.PORTO
FEUP FACULDADE DE ENGENHARIA
UNIVERSIDADE DO PORTO

ECCOMAS

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Implicit fully well-balanced methods for the shallow water model: a Lagrangian-Projection approach

C. Caballero-Cárdenas*, M. J. Castro-Díaz*, T. Morales de Luna* and M. L. Muñoz-Ruiz*

* Dpto. Analisis Matemático, Estadística e I. O. y Matemática Aplicada
Facultad de Ciencias, Universidad de Málaga
Málaga, Spain
e-mail: celiacaba@uma.es

Abstract: In a previous work, a family of well-balanced numerical methods was developed following a two-step algorithm called the Lagrange-Projection strategy, which exactly preserved the water at rest stationary solutions for the shallow water equations. Following this framework, we now present fully well-balanced finite volume numerical methods for approximating this equations and such that all the steady-states of the system are preserved: such kind of schemes are known as fully well-balanced. The algorithm consists of two steps. It first solves the shallow water system in Lagrangian coordinates: this is known as the Lagrangian step. Secondly, it projects the results onto Eulerian coordinates: this is what we call the Projection step. Concerning the time discretization, the Lagrangian step is treated implicitly, while the Projection step is done explicitly. This approach allows for decoupling of the acoustic and transport phenomena, which enables the use of larger time steps and reduces the restrictions imposed by the CFL condition.

Keywords: Fully well-balanced methods, Lagrange-Projection, implicit methods, shallow water model

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Deep Neural Network Approximation for Shape Uncertainty Quantification in Acoustic and Electromagnetic Scattering

Fernando Henriquez* **and Jürgen Dölz†**

* Chair of Computational Mathematics and Simulation Science (MCSS)
École Polytechnique Fédéral de Lausanne, Lausanne, Switzerland
Bâtiment MA, Station 8, CH-1015 Lausanne, Switzerland
e-mail: fernando.henriquez@epfl.ch

† Institute for Numerical Simulation
University of Bonn
Friedrich-Hirzebruch-Allee 7, 53115 Bonn, Germany
e-mail: doelz@ins.uni-bonn.de

Abstract: We consider the acoustic and electromagnetic scattering problems by random domains and surfaces. Our goal is to construct an efficient approximation of the corresponding domain-to-solution map. After considering a domain or surface parametrization depending on countably many parameters, one obtains a high-dimensional parametric map describing the problem's solution manifold. To tackle the efficient approximation of these maps, we adopt the approach proposed by Hesthaven and Ubbiali (Journal of Computational Physics 363 (2018): 55-78.). Firstly, by using a collection of so-called high-fidelity solutions or snapshots, a reduced basis is constructed to approximate the solution manifold. Then, we use deep feed-forward neural networks to compute the coefficient of the reduced basis solution. This procedure renders the evaluation of the approximate parameter-to-solution in the online phase independent of the offline part. Provided that the parameter-to-solution map satisfies certain smoothness properties, which have been verified for a range of models used in acoustic and electromagnetic scattering, we show that one can use quasi-Monte Carlo quadrature rules in the computation of the snapshots used in the reduced basis and also in the training of the involved deep neural networks. Finally, we provide numerical results for different models arising in acoustic and electromagnetic scattering

Keywords: Deep Neural Networks, Shape Uncertainty Quantification, Wave Scattering

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Real-time four-chamber heart electromechanical simulations enable effective clinical translation of computational cardiology

Salvador Matteo[1], Strocchi Marina[2], Regazzoni Francesco[3], Dede' Luca[3], Niederer Steven[2] and Quarteroni Alfio[3]

[1] Institute for Computational and Mathematical Engineering, Stanford University, California, USA

[2] Department of Biomedical Engineering, King's College London, London, UK

[3] MOX, Department of Mathematics, Politecnico di Milano, Milan, Italy

Abstract: In the framework of computational healthcare, developing faithful physics-based mathematical models of the cardiac function and efficient numerical methods is a major challenge for the scientific community. Nevertheless, the advent of novel Artificial Intelligence-based methods allows to create fast and accurate personalized heart models, which are essential for the advancement of treatment and surgical planning. We leverage Latent Neural Ordinary Differential Equations (LNODEs) to learn the temporal pressure-volume dynamics of a patient-specific four-chamber heart affected by ischemic cardiomyopathy. This surrogate model is trained from 400 3D-0D whole-heart closed-loop electromechanical simulations while spanning more than 40 model parameters, ranging from cardiac electromechanics to cardiovascular hemodynamics. LNODEs manifest a powerful representation of the 3D-0D model in a latent space by means of a feedforward fully-connected Artificial Neural Network that retains a very small amount of hyperparameters and allows for real-time numerical simulations of the cardiac function on a single processor. This surrogate model is employed to perform global sensitivity analysis and robust parameter estimation with uncertainty quantification in a few hours of computations. In particular, we match pressure and volume time traces unseen by LNODEs during the training phase and we calibrate tens of model parameters while also providing their posterior distribution.

Keywords: Cardiac Electromechanics, Machine Learning, Sensitivity Analysis, Parameter Estimation

1 Introduction

Detailed patient-specific cardiac simulations using accurate mathematical models can currently run on many cores of a supercomputer. In the framework of digital twinning and personalized medicine, bridging the chasm between the need for high-performance computing and the possibility of accurate real-time numerical simulations on a standard computer would have a tremendous impact on the future of cardiology [1]. In this work, we train a system of Latent Neural Ordinary Differential Equations (LNODEs) [2] that learns the pressure-volume loops of a heart failure patient while varying 43 model parameters of the whole cardiocirculatory function, by employing 400 3D-0D closed-loop electromechanical simulations [3]. We design a suitable loss function that guarantees excellent generalization properties of the trained feedforward fully-connected Artificial Neural Network (ANN) when the number of training samples is small compared to the dimensionality of the parameter space and the explored model variability. This ANN allows for real-time four-chamber

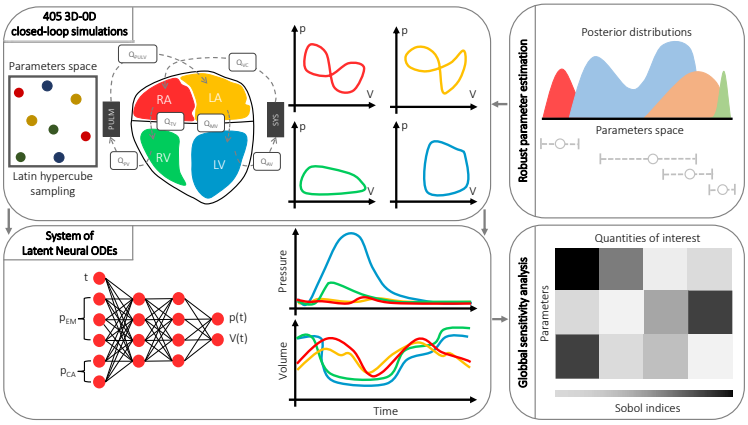


Figure 1: Sketch of the computational pipeline.

heart numerical simulations. We use LNODEs to perform global sensitivity analysis (GSA) and robust parameter estimation with uncertainty quantification (UQ) [1, 2]. We observe how model parameters impact the variability of scalar quantities of interest (QoIs) retrieved from the pressure-volume loops. We combine efficient matrix-free adjoint-based methods exploiting automatic differentiation and vectorization to calibrate tens of model parameters by matching the pressure and volume time traces coming from 5 unseen 3D-0D numerical simulations for the trained ANN.

2 Methods

We display the whole procedure in Figure 1. We perform 405 3D-0D closed-loop four-chamber heart electromechanical simulations. We build an accurate and efficient ANN-based surrogate model of the whole cardiovascular function by means of LNODEs. We carry out GSA to understand how each model parameter influences different QoIs extracted from the simulated pressure-volume loops. We robustly estimate many model parameters from time-dependent QoIs. Fully personalized 3D-0D numerical simulations can be performed after parameter calibration with UQ.

3 Conclusions

We propose a surrogate model based on LNODEs to learn the pressure-volume temporal dynamics of 3D-0D closed-loop electromechanical simulations. This surrogate model exploits a very lightweight feedforward fully-connected ANN containing a few neurons and hidden layers. LNODEs allow to encompass several applications of interest in a very fast and accurate manner by means of a small amount of computational resources. Indeed, running the training phase of the ANN along with GSA and robust parameter estimation on a single core standard laptop just require a few hours of computations.

References

[1] Salvador M, et al. Fast and robust parameter estimation with uncertainty quantification for the cardiac function. Comput Methods Programs Biomed 2023;231:107402.

[2] Regazzoni F, et al. A machine learning method for real-time numerical simulations of cardiac electromechanics. Comput Methods Appl Mech Eng 2022;393:114825.

[3] Strocchi M, et al. A publicly available virtual cohort of four-chamber heart meshes for cardiac electro-mechanics simulations. PLOS ONE 2020;15:1-26.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

How parametric uncertainty affects tipping points of the Atlantic meridional overturning circulation

Kerstin Lux*, Peter Ashwin†, Richard Wood‡, and Christian Kuehn*

* Department of Mathematics
School of Computation, Information and Technology, Technical University of Munich
Munich, Germany
e-mail: kerstin.lux@tum.de

† Department of Mathematics
University of Exeter
Exeter, United Kingdom

‡ Met Office Hadley Centre
Exeter, United Kingdom

Abstract: The Atlantic meridional overturning circulation (AMOC) has been identified as one of the Earth System Elements to be at risk of passing a tipping point (TP). This means it might undergo a critical transition passing from one stable state to a drastically different one under sustained anthropogenic forcing with severe consequences for the regulation of the North Atlantic heat transport. It is crucial to gain a deeper understanding of the underlying AMOC dynamics. We approach the tipping phenomenon via classical bifurcation theory. We model the AMOC in terms of a system of random Ordinary Differential Equations (RODEs), i.e. ODEs containing random parameters. The latter might be poorly known and the related uncertainty is inherited by the bifurcation curves and TPs themselves. Here, we contribute to an Uncertainty Quantification of AMOC tipping behavior by using a Bayesian parameter estimation technique. We are able to drastically constrain the tipping behavior. New visualization techniques are presented to highlight uncertain TP locations along the probabilistic bifurcation curve.

Keywords: Uncertainty Quantification, random ODEs, parametric uncertainty, bifurcations, tipping points

1 Introduction

In this talk, I will focus on results from our recent publication [1] and this extended abstract summarizes some of the key findings in [1].

The Atlantic meridional overturning circulation (AMOC) is considered to be at risk of tipping when threshold values of warming have been exceeded. Here, we work with rather simple AMOC models in terms of a system of Ordinary Differential Equations (ODEs).

One major challenge is that some model parameters are poorly known and we thus have to deal with parametric uncertainty in the models. This turns the original system of ODEs into random Ordinary Differential Equations (RODEs). Therefore, classical objects from bifurcation theory also become random such as bifurcation curves. While there is a rich theory of bifurcations and bifurcation curves for ODEs (see e.g. [4]) , much less is known for RODEs. For a more detailed overview of the topic, see [3].

2 Problem setup

In particular, we work with the two-box AMOC model presented in [2]. We use its known reduced dynamics on an attracting invariant manifold, which can be written together with the steady states (μ^*, x^*) as

$$\dot{x} = \mu - x\left(1 + \eta^2 (1-x)^2\right), \qquad \mu^* = x^*\left(1 + \eta^2 (1-x^*)^2\right). \tag{1}$$

where x represents the salinity difference, μ is proportional to the atmospheric freshwater flux, and the parameter η^2 gives the ratio of the diffusive to the advective timescale. The equilibria x^* interpreted as a function of μ depend crucially on the model parameter η^2, which is considered to be the uncertain parameter of interest.

We work with synthetic time series data of the salinity difference generated via a forward simulation of the ODE (1) with synthetic true values of $\eta^2 = 4$, $\mu = 0.85$, and $x_0 = 0.4$. We use the vector of every 100th simulated point with added Gaussian noise as data input $\hat{x}$ for the Bayesian inference.

3 Conclusions

By performing Bayesian inference on the model parameter η^2, we were able to substantially reduce the parametric uncertainty. In particular, this enables us to provide a more narrow range of tipping behavior. Our results contribute to an Uncertainty Quantification of high impact, low likelihood climate outcomes such as AMOC tipping and indicate that we might be able to use past knowledge to improve our understanding of likelihoods of future tipping events.

4 Acknowledgements

The authors acknowledge support of the EU within the TiPES project funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 820970. RW was also supported by the Met Office Hadley Centre Climate Programme, funded by BEIS.

References

[1] Lux K., Ashwin P., Wood R., Kuehn C. Assessing the impact of parametric uncertainty on tipping points of the Atlantic meridional overturning circulation. Environ. Res. Lett. 17.7 (2022), 075002.

[2] Cessi P. A simple box model of stochastically forced thermohaline flow. J. Phys. Oceanogr. (1994), 24 1911–20.

[3] Breden M., Kuehn C., Lux K. Nonlinear Dynamical Uncertainty Quantification for Random Differential Equations. In: SIAM DSWeb Issue: 2022, July.

[4] Kuznetsov Y. A. Elements of Applied Bifurcation Theory (2004) (Applied Mathematical Sciences vol 112) 3rd ed. New York: Springer.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A bi-fidelity collocation approach for kinetic epidemic models with random inputs

Bertaglia Giulia*, Liu Liu†, Pareschi Lorenzo‡ and Zhu Xueyu§

* Department of Environmental and Prevention Sciences
University of Ferrara, Ferrara, Italy
e-mail: giulia.bertaglia@unife.it

† Department of Mathematics
The Chinese University of Hong Kong, Shatin, N.T., Hong Kong SAR
e-mail: lliu@math.cuhk.edu.hk

* Department of Mathematics and Computer Science
University of Ferrara, Ferrara, Italy
e-mail: lorenzo.pareschi@unife.it

† Department of Mathematics
University of Iowa, Iowa City, IA, USA
e-mail: xueyu-zhu@uiowa.edu

Abstract: Data uncertainty is certainly one of the main problems in epidemiological modeling. The need for efficient methods capable of quantifying the effects of random inputs on outputs is essential to produce realistic scenarios of the spread of infection and to aim to implement the best control actions. In this work, we consider a bi-fidelity approach to quantify uncertainty in spatially dependent epidemic models. The approach is based on evaluating a high-fidelity model on a small number of samples appropriately selected on the basis of a large number of evaluations of a low-fidelity model, ensuring high computational efficiency and accuracy. In particular, we consider a class of multiscale kinetic transport models for high-fidelity reference and simple discrete-velocity kinetic models for low-fidelity evaluations. Both class of models share the same diffusive behavior and are solved numerically using methods that preserve their asymptotic limits, which permits to obtain stochastic asymptotic-preserving methods. A series of numerical experiments confirms the validity of the approach.

Keywords: Bi-Fidelity methods; Epidemic models; Kinetic transport equations; Stochastic Asymptotic-Preserving schemes; Uncertainty Quantification

1 Introduction

Amongst the various uncertainty quantification techniques, approaches based on non-intrusive stochastic strategies that do not necessarily require a priori knowledge of the probability density function (PDF) of uncertain parameters are particularly interesting in view of comparisons with experimental data, such as in the case of studies on the spread of infectious diseases. In this context, bi-fidelity (or multi-fidelity) methods represent an effective response, thanks to the adoption of control variate techniques based on the appropriate use of low-fidelity (LF) surrogate models, capable of accelerating the convergence of stochastic sampling.

2 Multiscale kinetic transport models for epidemics

We consider the class of multiscale kinetic system presented in [1] to describe an epidemic spread dynamics that takes into account the mobility of individuals and the presence of random inputs. To quantify the effects of these uncertainties following a bi-fidelity approach, the epidemic discrete-velocity kinetic system introduced in [2] is taken as reduced LF model. These models correctly describe the hyperbolic transport dynamics of the movement of individuals over long distances together with the small-scale diffusive nature typical of high-density urban areas, sharing the same diffusive limit. This allows for sufficient similarity in the model's random parameters space and enables the effectiveness of the following approach.

3 Asymptotic-preserving bi-fidelity collocation method

Considering a random input $z \in \Omega \subset \mathbb{R}$, the bi-fidelity collocation approach makes use of the solution of a computationally cheap LF model $u^{LF}(z)$ to effectively inform the selection of a small number of representative collocation points in the random parameter space. Thus, to construct accurate approximations of high-fidelity (HF) solutions $u^{HF}(z)$ evaluating the computationally expensive HF model only in a small number of selected samples, we build an inexpensive surrogate $u^{BF}(z)$ of the HF model in the following non-intrusive manner [3, 4]: $u^{HF}(z) \approx u^{BF}(z) = \sum_{k=1}^{N} c_k(z) u^{HF}(z_k)$, $z_k \in \gamma_N$, where N is the number of the selected collocation points in the parameter space $\gamma_N = \{z_1, \dots, z_N\}$. Here, these coefficients are acquired from the LF model, considering $c_k(z) \approx c_k^{LF}(z)$. Finally, to solve the systems at each collocation point, an asymptotic-preserving IMEX Finite Volume scheme that works uniformly in all regimes is adopted to obtain an efficient stochastic asymptotic-preserving method.

4 Conclusions

To examine the performance of the proposed methodology, several benchmark tests for different regimes are considered, which fully confirm the effectiveness of the approach.

References

[1] Bertaglia G, Boscheri W, Dimarco G, Pareschi L. Spatial spread of COVID-19 outbreak in Italy using multiscale kinetic transport equations with uncertainty. Math Biosci Eng 2021;18(5):7028–7059.

[2] Bertaglia G, Pareschi L. Hyperbolic compartmental models for epidemic spread on networks with uncertain data: Application to the emergence of COVID-19 in Italy. Math Models Methods Appl Sci 2021;31(12):2495–2531.

[3] Bertaglia G, Liu L, Pareschi L, Zhu X. Bi-fidelity stochastic collocation methods for epidemic transport models with uncertainties. Netw Heterog Media 2022;17(3):401–425.

[4] Liu L, Pareschi L, Zhu X. A bi-fidelity stochastic collocation method for transport equations with diffusive scaling and multi-dimensional random inputs. J Comput Phys 2022;462:111252.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Uncertainty quantification and predictability analysis of the Elder problem

Khotyachuk, Roman[1] **and Johannsen, Klaus**[2]

[1] The University of Bergen
Bergen, Norway
e-mail: roman.khotyachuk@uib.no

[2]NORCE Norwegian Research Centre AS
Bergen, Norway
e-mail: kljo@norceresearch.no

Abstract: This work is an attempt to investigate and understand a larger fraction of the full phase space of the Elder problem [1]. We sampled the phase space of the problem with a larger number of samples (10000 or even more perturbed solutions) with the aim of understanding the nonlinear dynamics and statistical properties of this problem using data-driven approaches [5]. Based on d3f PDE simulation software [4], Big Data technologies, and Machine Learning (ML) techniques, we achieved the following results:
— Analyzed statistical properties and the complexity of transient solutions regarding time, solution types, and other factors based on different complexity metrics;
— Investigated predictability of the Elder problem using ML classification methods [5] and estimated the time of 95% predictability.

Keywords: Elder problem, uncertainty quantification, data complexity, predictability

1 Introduction

The Elder problem [1, 2, 3], as a dynamical system described by the system of nonlinear PDEs of a parabolic type, is known to have three stable steady-state solutions called one-, two-, and tree-finger solutions (S1, S2, and S3 respectively). The system studied is unstable and very sensitive to even small perturbations in physical parameters, initial conditions, boundary conditions, etc. All these factors can change the dynamics of the studied process and lead to a steady state different from expected.

The main idea of this study is depicted in Figure 1, which is a visualization of one of the variables (features) used for predictive modeling (Section 3). This plot gives a 1-dimensional projection of the phase space of the Elder problem and allows us to consider the problem's dynamics in a simplified representation. We can see there multiple trajectories of perturbed solutions instead of three stable trajectories. These trajectories are quite similar in early time but diverge in a time of $t = 6...14$ years to three branches with S1, S2, or S3 solutions, respectively.

2 Analysis of transient solutions

We analyzed large ensembles of perturbed solutions to the Elder problem and calculated the statistical metrics of such ensembles. One important subtask in our study is to estimate the

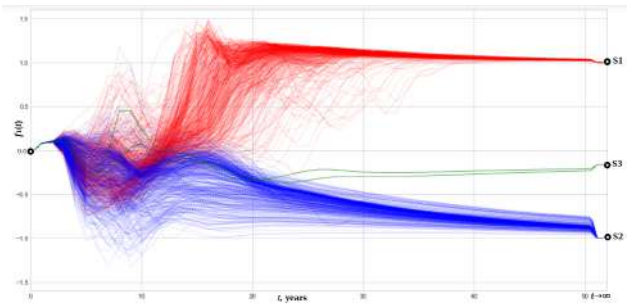


Figure 1: Visualization of the feature $F1$ in time for the ensemble of $N = 10000$ solutions.

number of "fingers" (concentration fields) in transient solutions at time t. To achieve this goal, we developed an approach based on averaging of solutions in a vertical (i.e., along the x-axis) direction. Furthermore, we analyzed the data complexity of solutions regarding time, solution types, and other factors using complexity metrics based on SVD [5], non-linearity, class overlapping, and other metrics [7]. We estimated the time of highest complexity ($t = 6–7$ years), which coincides with the time around $t = 6$ years indicated by Diersch and Kolditz in [3] as the most critical for the evolution of the process.

3 Predictability of steady-states

Steady-state prediction is important for a number of theoretical and practical cases when fingering is observed [3]. We developed several predictive models for the Elder problem using well-known classification methods [6] such as support vector machines (SVM), random forest (RF), and gradient boosting (GB) classifiers. These models are capable of predicting a steady state with acceptable accuracy and can be divided into three types as follows.

- Fully informed models (Type I);
- Partially informed models (Type II);
- Black-box models (Type III).

The best of our models can predict a steady state of the Elder problem with 95% accuracy at $t = 9 – 10$ years.

4 Conclusions

The presented results focused on the analysis of large ensembles of solutions to the Elder problem. This is made possible with our setup based on Big Data tools and data-driven approaches. We calculated the statistical metrics of transient solutions, investigated their complexity, and estimated the time of the highest complexity. We designed and evaluated three possible types of predictive models and their features and then estimated the prediction accuracy and the time of 95% predictability for the steady states of the problem. These results extend our knowledge of the Elder problem, especially about the properties of large ensembles of perturbed solutions.

References

[1] Elder, J.W. Transient convection in a porous medium. Journal of Fluid Mechanics, Volume 27, Issue 3, 24 February 1967, pp. 609 - 623. DOI: https://doi.org/10.1017/S0022112067000576.

[2] Simmons, C.T. and Elder, J.W. The Elder Problem. Groundwater, **2017**, Vol. 55, 926–930. https://doi.org/10.1111/gwat.12593.

[3] Diersch, J.G.; Kolditz, O. Variable-density flow and transport in porous media: approaches and challenges. Advances in water resources, **2002**, 25, pp. 899–944. DOI: 10.1016/S0309-1708(02)00063-5.

[4] Fein, E. d3f – ein Programmpaket zur Modellierung von dichtegetriebenen Strömungen. GRS, Braunschweig, GRS-139, **1998**, ISBN 3-923875-97-5.

[5] Kutz, J. N. Data-Driven Modeling & Scientific Computation: Methods for Complex Systems & Big Data. **2013**. Oxford University Press. ISBN 978-0-19-966034-6.

[6] Data Classification: Algorithms and Applications. Aggarwal, C. (Editor). Chapman & Hall/CRC, 2014. ISBN-10: 1466586745.

[7] Lorena, A., Garcia, L., Lehmann, J., Pereira de Souto, M.C., Ho, T. How Complex is your classification problem? A survey on measuring classification complexity. ACM Computing Surveys (CSUR), **2018**, vol. 52, pp. 1 -34. https://doi.org/10.1145/3347711.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Dynamical Low Rank Approximations: SUPG stabilisation and time-stepping schemes

Yoshihito Kazashi[†], Fabio Nobile[*], Thomas Trigo Trindade[*], Eva Vidličková

[†] Institute of Applied Mathematics and
Interdisciplinary Center for Scientific Computing (IWR)
Heidelberg University

[*] Department of Mathematics, CSQI
EPFL, Switzerland
e-mail: {fabio.nobile,thomas.trigotrindade}@epfl.ch

Abstract: The Dynamical Low Rank (DLR) method is a time-dependent reduced basis method attractive for the quantification of uncertainties of time-dependent random PDEs for which the optimal low-rank subspace may vary significantly over time. The true solution is approximated by an expansion of deterministic modes weighted by stochastic coefficients, all time-dependent, and for which evolution equations are available. The analysis of time-integration schemes is complicated by the fact that the updated solution is obtained in a non-linear fashion. Recently, we have shown that a projector-splitting scheme, combined with standard first-order time integration of the operator, leads to a fully discrete DLR solution verifying a variational formulation. This tool allows us to show that certain norm-bound properties of the full order model are recovered by the DLR solution. In this talk, we propose extensions of the projector-splitting scheme, including a practical Strang scheme as well as other time-marching schemes which improve on the accuracy of the approximation and its numerical stability compared to explicit integrators while not being overly expensive. Furthermore, we derive SUPG-stabilised DLR equations for advection-dominated problems. The numerical solution is shown to verify a variational formulation on a "skewed" testing space, which we use to obtain standard norm-stability estimates of the numerical solution.

Keywords: Dynamical Low-Rank Approximations, Petrov-Galerkin, Uncertainty Quantification, Stabilisation of Advection-Dominated Problems

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Shape uncertainty quantification with localized basis functions

van Harten, Wouter[†] **and Scarabosio, Laura**[*]

[†] Institute for Mathematics, Astrophysics, and Particle Physics (IMAPP)
Radboud University
Nijmegen, The Netherlands
w.vanharten@math.ru.nl

[*] Institute for Mathematics, Astrophysics, and Particle Physics (IMAPP)
Radboud University
Nijmegen, The Netherlands
l.scarabosio@math.ru.nl

Abstract: In this talk, we consider a linear, elliptic, partial differential equation (PDE) on a domain $D(\boldsymbol{y})$ where the domain is parametrized by $\boldsymbol{y} \in [-1,1]^d$, d possibly countably infinite. Polynomial expansions of parametric linear elliptic PDEs recently got a lot of attention when first, it was shown that these expansions converge at least with a rate $1/p - 1$, when $(\|\psi_j\|_\infty)_{j\in\mathbb{N}} \in \ell^p$ and therefore, the convergence does not suffer from the curse of dimensionality. Later, for affine parametric diffusion coefficient $a(\boldsymbol{y})$, faster convergence rates were observed and proven for wavelet-type expansions by utilizing a pointwise bound on $(\psi_j)_{j\in\mathbb{N}}$ instead of the previously exploited L^∞-bound. In this work, we expand these results to the linear elliptic equation with parametrized boundary by employing a mapping approach to handle the parametrized domain. In particular, we show theoretically and illustrate numerically that locality in the support of the functions allows us to achieve higher convergence rates than globally supported basis functions.

Keywords: Domain uncertainty, Mapping approach, Parameter-to-solution map, Surrogate model, Polynomial approximation

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Hierarchical Sampling Techniques and Goal-Oriented Adaptive Finite Element for Elliptic PDE with Lognormal Coefficients

Joakim Beck*, Yang Liu*, Erik von Schwerin* and Raul Tempone*,†

* Computer, Electrical and Mathematical Sciences and Engineering Division
King Abdullah University of Science and Technology (KAUST)
Thuwal 23955-6900, KINGDOM OF SAUDI ARABIA.
e-mail: {joakim.beck, yang.liu.3, erik.vonschwerin, raul.tempone}@kaust.edu.sa

† Alexander von Humboldt Professor in Mathematics for Uncertainty Quantification
RWTH Aachen University, 52062 Aachen, GERMANY.
e-mail: tempone@uq.rwth-aachen.de

Abstract: We present an adaptive multilevel Monte Carlo (AMLMC) algorithm [1] for approximating deterministic, real-valued, bounded linear functionals that depend on the solution of a linear elliptic PDE with a lognormal diffusivity coefficient and geometric singularities in bounded domains. Our AMLMC algorithm is built on the dual-weighted-residual error representation. To suit the geometric nature of the singularities in the solution, our AMLMC algorithm uses a sequence of deterministic, non-uniform auxiliary meshes as a building block. This adaptive approach is particularly useful for the lognormal case treated here, which lacks uniform coercivity and thus produces functional outputs that vary over orders of magnitude. Furthermore, we discuss iterative solvers and compare their efficiency with direct ones. To reduce computational work, we propose a stopping criterion for the iterative solver with respect to the quantity of interest, the realization of the diffusivity coefficient, and the desired level of AMLMC approximation.

Keywords: Multilevel Monte Carlo, Goal-oriented adaptivity, Computational complexity, Finite elements, Partial differential equations with random data, Lognormal diffusion

1 Introduction

We consider the adaptive computation and error control for quantities of interest (QoIs) of the form $\mathbb{E}[Q(u)]$, where Q is a deterministic, real-valued, bounded linear functional of the stochastic solution u to a class of linear elliptic PDE with random coefficients,

$$-\nabla \cdot (a(\mathbf{x};\omega)\nabla u(\mathbf{x};\omega)) = f(\mathbf{x};\omega) \qquad \text{for } \mathbf{x} \in \mathcal{D}, \tag{1a}$$

$$u(\mathbf{x};\omega) = 0 \qquad \text{for } \mathbf{x} \in \partial\mathcal{D}_1, \tag{1b}$$

$$\partial_n u(\mathbf{x};\omega) = 0 \qquad \text{for } \mathbf{x} \in \partial\mathcal{D} - \partial\mathcal{D}_1, \tag{1c}$$

where the differential operators, $\nabla\cdot$ and ∇, are taken with respect to the spatial variable, $\mathbf{x}$. Here, ω corresponds to a complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$. With respect to the spatial domain $\mathcal{D}$, an open and bounded polygonal/polyhedral domain in $\mathbb{R}^d$, $d \geq 2$.

2 Adaptive Multilevel Monte Carlo

MLMC uses hierarchical control variates to substantially reduce the computational cost of MC. Thus, it uses a hierarchy of $L+1$ meshes defined by decreasing mesh sizes, indexed by

their levels $\ell = 0, 1, \ldots, L$, and the telescopic representation of the expected value of the finest approximation. Thus, letting Q_ℓ denote the approximation of Q on level ℓ,

$$\mathbb{E}[Q_L] = \mathbb{E}[Q_0] + \sum_{\ell=1}^{L} \mathbb{E}[Q_\ell - Q_{\ell-1}].$$

$$\mathcal{A}_{MLMC} = \frac{1}{M_0} \sum_{n=1}^{M_0} Q_0(\omega_{0,n}) + \sum_{\ell=1}^{L} \frac{1}{M_\ell} \sum_{n=1}^{M_\ell} \left(Q_\ell(\omega_{\ell,n}) - Q_{\ell-1}(\omega_{\ell,n}) \right), \tag{2}$$

where $\{\omega_{\ell,n}\}_{n=1,\ldots,M_\ell}^{\ell=0,\ldots,L}$ denote i.i.d. realizations of the mesh-independent random variables. In MLMC, it is fundamental to evaluate both terms in the difference

$$\Delta Q_\ell(\omega_{\ell,n}) = Q_\ell(\omega_{\ell,n}) - Q_{\ell-1}(\omega_{\ell,n}) \tag{3}$$

with the same outcome of $\omega_{\ell,n}$.

Algorithm 1 computes one sample of level ℓ in AMLMC. The factor $K_k(\omega)$ involved in the stopping criterion, is given by $\frac{\int_{\mathcal{D}} \tilde{\rho}_k(x;\omega)^{\frac{1}{2}}\, dx}{\int_{\mathcal{D}} \mathbb{E}\left[\rho^{\frac{1}{2}}\right]}$, where $\tilde{\rho}_k(x;\omega)$ is the approximated error density on mesh k with sample ω.

Algorithm 1 One sample of $\Delta Q_\ell = Q_\ell - Q_{\ell-1}$

Set $k = 0$, errest $= +\infty$, $CoarseFlag = true$
Sample the R.V. defining the field $\overline{a}$
while *true* **do**
    Evaluate the random field $\bar{a}_k$ on mesh $\mathcal{H}_k$
    if $\ell = 0$ **then**
        Set $Q_{\ell-1} = 0$
        Set $CoarseFlag = false$
    end if
    if errest $< K_k(\omega) \cdot \mathrm{TOL}_{\mathrm{bias},\ell-1} \wedge CoarseFlag$ **then**
        Set $Q_{\ell-1} = (g * \mathbf{1}_{D_0}, u_{k,*})$
        Set $CoarseFlag = false$
    end if
    if errest $< K_k(\omega) \cdot \mathrm{TOL}_{\mathrm{bias},\ell}$ **then**
        Set $Q_\ell = (g * \mathbf{1}_{D_0}, u_{k,*})$
        break;
    end if
    Set $k = k + 1$
end while

References

[1] Beck J, Liu Y, von Schwerin E, Tempone R. Goal-Oriented Adaptive Finite Element Multilevel Monte Carlo with Convergence Rates. Computer Methods in Applied Mechanics and Engineering 2022;402:115582.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Convergence of adaptive empirical stochastic Galerkin FEM

Martin Eigel[*], **Nando Farchmin**[†]

[*] Weierstrass Institute (WIAS)
Berlin, Germany
e-mail: eigel@wias-berlin.de

[†] Physikalisch Technische Bundesanstalt (PTB)
Berlin, Germany
e-mail: nando.farchmin@ptb.de

Abstract: Adaptive stochastic Galerkin FEM (ASGFEM) with residual based a posteriori error estimation allow for near optimal convergence in practice for common parametric linear PDEs. However, their implementation is rather involved and requires significant effort when different types of PDEs should be tackled. Motivated by recent results with empirical low-rank tensor regression in the framework of statistical learning, we propose a non-intrusive reconstruction method that only uses samples of the solution and yields the Galerkin projection with high probability. As a new result we show that the adaptive algorithm converges even for non-affine coefficients.

Keywords: parametric PDE, tensor reconstruction, error estimation, adaptivity, stochastic FEM

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Uncertainty quantification for diffusion problems using the data-driven approach

Adriana Kuliková[1*], Andrei G. Shvarts[1], Łukasz Kaczmarczyk[1] and Chris J. Pearce[1]

[1] Glasgow Computational Engineering Centre (GCEC)
James Watt School of Engineering, University of Glasgow, Glasgow, UK
e-mail: a.kulikova.1@research.gla.ac.uk

Abstract: We apply the Data-Driven approach to diffusion problems: the conservation laws and boundary conditions are satisfied by means of the finite element method, while a dataset is used directly in simulations, avoiding the need of fitting material model parameters. The weaker mixed formulation provides *a posteriori* error estimates used for adaptive *hp*-refinement, reducing the number of unknowns for the desired accuracy and, consequently, the number of searches through the material dataset. Therefore, we can use Monte-Carlo analysis to provide the information about uncertainty of the results alongside the solution of the problem.

Keywords: Data-driven mechanics, Mixed formulation, Adaptive refinement, Uncertainty quantification

1 Introduction

The Data-Driven (DD) approach aims to abandon the fitting and use (noisy) material data directly in simulations, while satisfying the conservation laws and boundary conditions by e.g. the finite element method [1]. In this work we develop DD framework for diffusion problems derived with the weaker mixed formulation, which is natural for the considered physics as it enforces continuity of the normal flux component across any inner boundaries [2]. Furthermore, such formulation allows for an adaptive *hp*-refinement, permitting to minimise the volume of computations needed for a given accuracy and use a statistical method such as Monte-Carlo to quantify the uncertainty of the results. The developed DD framework has been implemented using an open-source parallel finite element library MoFEM [3].

2 Mixed data-driven formulation for diffusion problems

DD approach avoids material models and uses instead material datasets containing points with gradient of pressure $\mathbf{g} = \nabla p$ and flux $\mathbf{q}$ in case of diffusion problems. The solution is achieved through an iterative process of finding the closest points in the material dataset for the values of unknown fields at every integration point in the domain, which are found from a global FEM analysis. The FEM formulation is based on minimising a functional quantifying the distance between the unknown field values and the material dataset $J(\mathbf{g}, \mathbf{q})$ and imposing constraints for conservation law $\nabla \cdot \mathbf{q} = f$ and the relation $\mathbf{g} = \nabla p$. After integration by parts and application of boundary conditions ($\mathbf{q} \cdot \mathbf{n} = \bar{q}$ on Γ_q and $p = \bar{p}$ on Γ_p), the Lagrangian reads:

$$\mathcal{L}(p, \mathbf{g}, \mathbf{q}, \boldsymbol{\tau}, \lambda) = J(\mathbf{g}, \mathbf{q}) + \int_\Omega \boldsymbol{\tau} \cdot \mathbf{g} \, d\Omega - \int_{\Gamma_p} (\boldsymbol{\tau} \cdot \mathbf{n}) \bar{p} \, d\Gamma + \int_\Omega (\nabla \cdot \boldsymbol{\tau}) p \, d\Omega + \int_\Omega \lambda (\nabla \cdot \mathbf{q}) \, d\Omega - \int_\Omega \lambda f \, d\Omega, \quad (1)$$

where λ and $\boldsymbol{\tau}$ are scalar and vector Lagrange multipliers, respectively, and the unknown functions are in following spaces: $p, \lambda \in L^2(\Omega)$, $\mathbf{g} \in \mathbf{L}^2(\Omega)$, $\mathbf{q}, \boldsymbol{\tau} \in H(\mathrm{div}; \Omega)$. Weaker mixed

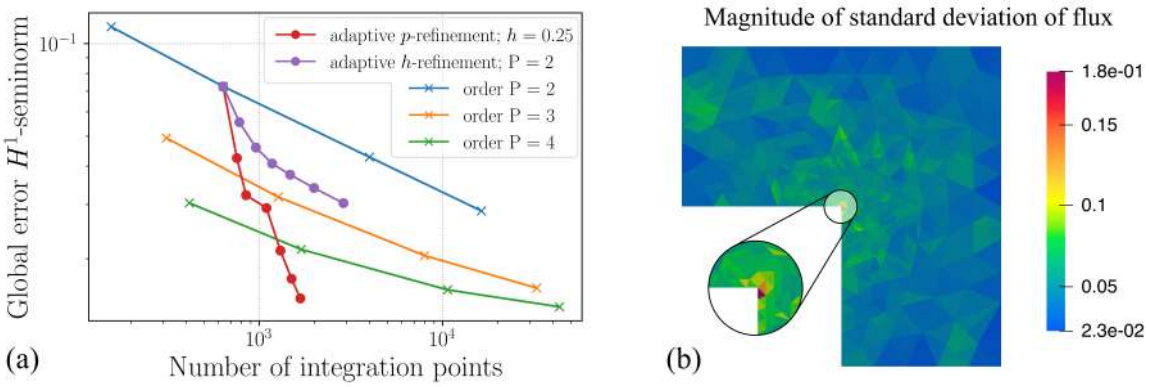


Figure 1: L-shape domain results: (a) H^1-seminorm convergence, (b) standard deviation of the solution.

DD formulation (1) allows for naturally emerging *a posteriori* error indicators/estimators, e.g. $\eta_e(\nabla p, \mathbf{g}) = ||\nabla p - \mathbf{g}||^2_{\Omega_e}$, according to which adaptive *hp*-refinement takes place, see Fig. 1(a).

3 Uncertainty quantification

While FE error can be controlled using the adaptive refinement, the results presented in Fig. 1(a) possess uncertainty due to the noise in a material dataset. Moreover, the solution is not unique and depends of the initial values of the unknown fields. Therefore, the uncertainty of the results can be quantified by statistical methods such as Monte-Carlo analysis. Fig. 1(b) shows the distribution of the standard deviation associated with the flux part of the solution.

4 Conclusions

The weaker mixed formulation for the data-driven approach provides error indicators which are used for adaptive *hp*-refinement. Furthermore, Monte-Carlo analysis is performed with the smallest number of DOFs for a given accuracy, to quantify the uncertainty associated with the solution using the associated (noisy) material dataset.

5 Acknowledgements

This work was supported by EDF and EPSRC. The views expressed in this paper are those of the authors and not necessarily those of EDF.

References

[1] T. Kirchdoerfer, M. Ortiz (2016): Data-driven computational mechanics. *Computer Methods in Applied Mechanics and Engineering* 304, 81-101.

[2] D. Boffi, F. Brezzi, M. Fortin et al. (2013): Mixed finite element methods and applications. *Springer*, vol. 44.

[3] Ł. Kaczmarczyk et al. (2020): MoFEM: An open source, parallel finite element library. *Journal of Open Source Software*, 5(45), 1441.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Efficient solution of the covariance eigenvalue problem for stationary random fields

Chao Zhang*, Oliver Ernst†

* Department of Mathematics
Chemnitz University of Technology
Chemnitz, Germany
e-mail: chao.zhang@math.tu-chemnitz.de

† Department of Mathematics
Chemnitz University of Technology
Chemnitz, Germany
e-mail: oernst@math.tu-chemnitz.de

Abstract: The Karhunen-Loève expansion has been a common approach in approximating random fields, but the solution of the underlying Fredholm integral eigenvalue problem for large-scale problems is challenging. In this work, we describe a numerical solution approach for efficiently approximating the dominant eigenpairs of the covariance operator of stationary random fields. The methods combine advanced quadrature from the boundary element method with fast matrix-vector multiplication based on hierarchical matrix approximation as well as the thick-restart Lanczos process for approximating eigenpairs. Firstly, we employ the Sauter-Schwab quadrature scheme for accurate evaluation of the double integrals from discretizing the kernel operator with the Galerkin method. The Sauter-Schwab scheme alleviates the singularity of the integrals in the case of coincident, common-edge, and common-vertex elements. Secondly, The hierarchical matrix is adopted to approximate the Galerkin system matrix. By replacing far-field blocks of a matrix by inexpensive low-rank approximations, this technique allows us to efficiently store the dense matrix and effect its action on a vector. Krylov-based methods are finally used to solve the resulting eigenvalue problem. Numerical results demonstrate the effectiveness of a combined use of the above techniques in approximating random fields.

Keywords: Random fields, Karhunen-Loève expansion, Boundary element method, Hierarchical matrices, Thick-restart Lanczos method

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Bayesian inverse problems for hyperbolic conservation laws

Masoumeh Dashti* **and Duc-Lam Duong†**

* Department of Mathematics
School of Mathematical and Physical Sciences, University of Sussex
Brighton, UK
e-mail: m.dashti@sussex.ac.uk

† Department of Computational Engineering
School of Engineering Science, LUT University
Lappeenranta, Finland
e-mail: duc-lam.duong@lut.fi

Abstract: We consider the inverse problem of recovering the upstream field or the flux function of a scalar conservation law from discrete pointwise measurements of the particle trajectories that are moving along the flow. These types of inverse problems in the context of hyperbolic conservation laws are challenging due to discontinuities (shockwaves) in the solution. We employ the Filippov theory of differential equations to study the existence, uniqueness and stability of the trajectories. We show that such a Filippov solution can be obtained via front tracking and vanishing viscosity approximations and that the approximate trajectories given by either of these methods converge uniformly. For certain classes of flux functions, illustrated by traffic flow, we prove the Hölder continuity of the particle trajectories with respect to the initial field or the flux function. We show that the above continuity properties translate to the stability of the Bayesian regularised solutions of the inverse problems with respect to appropriate approximations of the forward map.

Keywords: Scalar conservation laws, traffic flow, Bayesian inverse problems, uncertainty quantification.

1 Introduction

Let us consider the Cauchy problem for scalar conservation laws

$$\partial_t \rho(x,t) + \partial_x f(\rho(x,t)) = 0, \quad x \in \mathbb{R},\ t > 0, \tag{1}$$

$$\rho(x,0) = \rho_0(x), \quad x \in \mathbb{R}, \tag{2}$$

where $\rho : \mathbb{R} \times [0,\infty) \to \mathbb{R}$ is the density of some conserved physical quantity, and $f : \mathbb{R} \to \mathbb{R}$ represents its flux. We are interested in the inverse problems of recovering the initial field ρ_0 or the flux function f from observations of the solution ρ. These kinds of inverse problems, even though challenging (due to shockwaves and irreversibility in the forward problem [1]), have many applications, for example in the case of traffic flow, they correspond to the problems of determining the upstream vehicle density or the flux given finite observations of the traffic at later times. The inverse problems can be written as

$$y = G(u) + \xi, \tag{3}$$

where u is either ρ_0 or f, y is the observed data and G is the observation map which is defined via the solution of the forward problem. We consider the observation map as $G(u) = \{z(t_j)\}_{j\in J}$, for some finite index sets J, where z is a particle trajectory corresponding to the entropy solution of the conservation law (1).

2 Stability of the forward problem

We denote by $w = w(\rho)$ the velocity of the flow. The trajectory $z(t)$ of a particle starting from x_0 is then defined by the ODE

$$\dot{z}(t) = w(\rho(z(t), t)), \quad z(t_0) = x_0. \tag{4}$$

Since ρ is typically a discontinuous function of both z and t, a solution to (4) is understood in the sense of Filippov. We have the following stability result [2].

Theorem 2.1 *Let $0 < m_\rho < 1$ and $T > 0$ be given. Suppose that ρ and $\bar{\rho}$ are solutions to (1)-(2) with initial values $\rho_0, \bar{\rho}_0 \in L^1 \cap BV(\mathbb{R}; [m_\rho, 1])$ respectively, satisfying $\|\rho_0 - \bar{\rho}_0\|_{L^1 \cap L^\infty(\mathbb{R})} \leq \varepsilon$. Let z and $\bar{z}$ be the corresponding particle trajectories with the same initial position x_0. Then $\|z - \bar{z}\|_{L^\infty([t_0,T])} \leq C_\rho \, \varepsilon^{1/2}$, with $C_\rho = 1 + (T - t_0)(1 + \frac{2}{m_\rho})L_w + \frac{1}{m_\rho}(\|\rho_0\|_{BV} + \|\bar{\rho}_0\|_{BV})$.*

3 Solutions to the Bayesian inverse problems

By adapting a Bayesian framework [3], we are able to show that, not only the posterior is well-defined and continuous in data, it is stable w.r.t perturbations in the forward map [2].

Theorem 3.1 *Suppose $y \in \mathbb{R}^J$ is given by (3). Let μ_0 be a prior probability measure on X where $X = L^1(\mathbb{R}) \cap BV(\mathbb{R})$. Then the posterior measure μ^y given by*

$$\frac{d\mu^y}{d\mu_0}(u) = \frac{1}{Z} \exp \fint \frac{1}{2\gamma^2} |y - G(u)|^2),$$

with $Z = \int_X \exp \fint \frac{1}{2\gamma^2} |y - G(u)|^2) \, d\mu_0$ is well-defined and continuous in Hellinger distance w.r.t. y.

Theorem 3.2 *Let $X = L^1 \cap BV(\mathbb{R}; (0, 1))$. Suppose that for any $u, u^N \in X$ that satisfy*

$$\|u^N - u\|_{L^1 \cap L^\infty} \leq \psi(N), \quad \psi(N) \to 0 \text{ as } N \to \infty.$$

Assume that $\mu_0(X) = 1$, and $\frac{1 + \|u\|_{BV}^2}{m_u^2} \in L^1_{\mu_0}(X)$ where $m_u = \inf_{x \in \mathbb{R}} u(x)$. Then, the corresponding postoriors μ and μ^N satisfy, as $N \to \infty$,

$$d_{\text{Hell}}(\mu^N, \mu) \leq C \sqrt{\psi(N)}.$$

We note that, stability in other metrics, such as Wasserstein distance, may be obtained as well [4] (see also related discussions in [5]).

References

[1] C.M. Dafermos, *Hyperbolic Conservation Laws in Continuum Physics*, 4th ed., Springer, 2016.

[2] M. Dashti, D.-L. Duong, *Stability of particle trajectories of scalar conservation laws and applications in Bayesian inverse problems*, 2022, submitted.

[3] A.M. Stuart, *Inverse problems: a Bayesian perspective*, Acta Numerica, 19 (2010), 451–559.

[4] D.-L. Duong, *Inverse problems for hyperbolic conservation laws: a Bayesian approach*, PhD thesis, University of Sussex, 2021.

[5] B. Sprungk. *On the local Lipschitz stability of Bayesian inverse problems.* Inverse Problems 36, no. 5 (2020): 055015.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Subsampling in Ensemble Kalman Inversion

Hanu Matei*, Latz Jonas† and Schillings Claudia‡

* Institut für Mathematik
Freie Universität Berlin (FU Berlin)
Berlin, Germany
e-mail: matei.hanu@fu-berlin.de

† School of Mathematical and Computer Sciences
Department of Actuarial Mathematics and Statistics
Heriot-Watt University
Edinburgh, UK
e-mail: j.latz@hw.ac.uk

‡ Institut für Mathematik
Freie Universität Berlin (FU Berlin)
Berlin, Germany
e-mail: c.schillings@fu-berlin.de

Abstract: Inverse problems seek to find parameters that generate a set of observed data in a mathematical model. Several methods have been proposed to solve inverse problems such are optimisation and Bayesian approaches. In this talk, we consider the Ensemble Kalman Inversion (EKI) which has been recently introduced as an efficient, gradient-free method. Based on the continuous-time Ensemble Kalman Filter, it uses an ensemble of particles and a linearisation technique to essentially estimate the posterior distribution in an underlying Bayesian inverse problem. Unfortunately, the algorithm becomes inefficient or even computationally infeasible if the considered data set is too large. A similar problem appears in large-scale optimisation with gradient descent algorithms in, e.g., machine learning. Here, randomised algorithms like stochastic gradient descent (SGD) have become popular: those use only a random subset of the data in each iteration. These are so-called subsampling techniques. In the past, subsampling has been employed in the EKI, but not analysed. Based on a recent analysis of a continuous-time representation of SGD, we propose, analyse, and apply a subsampling-technique within EKI. Indeed, we propose two different subsampling techniques: either every particle observes the same data subset (single subsampling) or every particle observes a different data subset (batch subsampling).

Keywords: Inverse Problems, Ensemble Kalman Inversion, Subsampling, Continuos time Markov processes

References

[1] Neil K. Chada, Andrew M. Stuart, and Xin T. Tong. Tikhonov regularization within ensemble kalman inversion. *SIAM Journal on Numerical Analysis*, 58(2):1263–1294, 2020.

[2] Jonas Latz. Analysis of stochastic gradient descent in continuous time. *Statistics and Computing*, 31:39, 2021.

[3] Claudia Schillings and Andrew M. Stuart. Analysis of the ensemble kalman filter for inverse problems, 2016.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Learning the noise parameters of Bayesian inverse problems using normalizing flows

Paul Hagemann*, Johannes Hertrich* and Gabriele Steidl*

* Technische Universität Berlin Berlin, Germany e-mail:hagemann@math.tu-berlin.de

Abstract: In this talk I will outline the basics of conditional normalizing flows to solve Bayesian inverse problems. First the basics of optimization such as forward and reverse Kullback-Leibler divergence will be discussed. Then special attention will be drawn to a very specific noise model, namely mixed (both additive and multiplicative noise). This will be learned jointly with the posterior, by iteratively updating the estimated posterior of Bayesian inverse problems and the noise parameters. This will be embedded into the theoretical framework of EM algorithms in order to present convergence results. Finally applications to inverse problems will be shown.

Keywords: Inverse Problems, Normalizing Flows, Uncertainty Quantification

1 Extended abstract

Recently, there have been a number of papers applying conditional normalizing flows to solve Bayesian inverse problems [1, 3, 9, 2, 6]. The general idea is to establish a family of paramterized diffeomorphisms $T(y)$, where $y = f(x) + \xi$ with f as the forward operator, ξ as the error model and y as the measurement. Usually, they are trained on a loss of the form $E_y \not\oint \mathrm{KL}(p_{x|y}, T(y)_\# p_z)$, which penalizes the distance between the posterior and the pushforward of the conditional generative model.

In this talk we will consider a very specific noise model [4], i.e. mixed noise. Here the noise parameter ξ will consists of an additive and a multiplicative component, i.e. $\xi \sim \mathcal{N}(0, a^2 f(x)^2 + b^2)$ for constants a and b. This noise model has some relevance in physics [7, 8] applications, where some error scales with the intensity and the other is background noise. We will outline a framework on how to jointly learn a conditional generative model to sample from the posterior as well as the noise parameters a and b. Our algorithm consists of two basics steps at step n.

For this we define $\int_{\mathbb{R}^d} \log\left(\frac{p_{X_\theta, Y_\theta}(x,y)}{q(x)}\right) q(x)dx = \mathcal{F}(q, \theta|y)$, where $q = T(y)_\# p_z$ in our setting and $\theta = (a, b)$.

- Update the estimated posterior by maximizing $\mathcal{F}(q, a^n, b^n|y)$ for randomly drawn y according to a^n and b^n.
- Update a and b by maximizing $\mathcal{F}(q, a, b|y)$ for fixed q.

Convergence results and applications to imaging and physical inverse problems will be discussed and outlined. However, this setting is not limited to learning noise parameters as demonstrated in [5].

References

[1] A. Andrle, N. Farchmin, P. Hagemann, S. Heidenreich, V. Soltwisch, and G. Steidl. Invertible neural networks versus mcmc for posterior reconstruction in grazing incidence x-ray fluorescence. In *International Conference on Scale Space and Variational Methods in Computer Vision*, pages 528–539. Springer, 2021.

[2] L. Ardizzone, C. Lüth, J. Kruse, C. Rother, and U. Köthe. Guided image generation with conditional invertible neural networks. *ArXiv:1907.02392*, 2019.

[3] A. Denker, M. Schmidt, J. Leuschner, and P. Maass. Conditional invertible neural networks for medical imaging. *Journal of Imaging*, 7(11):243, 2021.

[4] M. M. Dunlop. Multiplicative noise in bayesian inverse problems: Well-posedness and consistency of map estimators, 2019.

[5] A. F. Gao, J. C. Castellanos, Y. Yue, Z. E. Ross, and K. Bouman. DeepGEM: Generalized expectation-maximization for blind inversion. In A. Beygelzimer, Y. Dauphin, P. Liang, and J. W. Vaughan, editors, *Advances in Neural Information Processing Systems*, 2021.

[6] P. Hagemann, J. Hertrich, and G. Steidl. Stochastic normalizing flows for inverse problems: a markov chains viewpoint. *arXiv preprint arXiv:2109.11375*, 2021.

[7] S. Heidenreich, H. Gross, and M. Bär. Bayesian approach to the statistical inverse problem of scatterometry: Comparison of three surrogate models. *Int. J. Uncertain. Quantif.*, 5(6), 2015.

[8] S. Heidenreich, H. Gross, and M. Bär. Bayesian approach to determine critical dimensions from scatterometric measurements. *Metrologia*, 55(6):S201, Dec. 2018.

[9] J. Kruse, G. Detommaso, R. Scheichl, and U. Köthe. HINT: Hierarchical invertible neural transport for density estimation and Bayesian inference. *ArXiv:1905.10687*, 2020.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Langevin dynamics: Enrichment and Homotopy

Martin Eigel*, Robert Gruhlke† and Claudia Schillings† and David Sommer*

† Institut für Mathematik, FU Berlin
Arnimallee 6, 213,
14195 Berlin, Germany
e-mail: r.gruhlke@fu-berlin.de
c.schillings@fu-berlin.de

* Weierstrass Institute,
Mohrenstr. 39,
10117 Berlin, Germany
e-mail: eigel@wias-berlin.de
sommer@wias-berlin.de

Abstract: In this work we present recent enhancements of covariance preconditioned state-of-the-art Langevin samplers through the introduction of ensemble enrichment and homotopy. The first approach addresses the reduction of effective function calls of the underlying potential in the deterministic drift term of the particle system. This becomes highly relevant, when Langevin samplers are used for the solution of Bayesian inference problems, and the potential is defined upon a forward model. In the second approach the drift term of the Langevin dynamics becomes time-inhomogeneous, directing the overall particle system along intermediate measures towards the target distribution. Numerical results demonstrate the efficiency of both techniques, including fast convergence in the case of multi-modal posterior distributions.

Keywords: Bayesian inference, Langevin Dynamics, Particle Systems, Homotopy

1 Introduction

Consider the inverse problem of finding an unknown $y \in \mathbb{R}^D$ from an observation $\Delta \in \mathbb{R}^K$ for $D, K \in \mathbb{N}$, where

$$\Delta = \mathcal{G}(y) + \eta, \tag{1}$$

with a deterministic forward operator $\mathcal{G}\colon \mathbb{R}^D \to \mathbb{R}^K$ and centered Gaussian observational noise $\eta \sim \mathcal{N}(0, \Gamma)$ with positive definite covariance matrix $\Gamma \in \mathbb{R}^{K,K}$. In the Bayesian framework, a prior distribution μ_{prior} is associated with the unknown y. Then, for a given measurement $\Delta = \tilde{\Delta}$, the prior is updated via Bayes' rule to yield a posterior distribution μ_*. Here, we assume that μ_{prior} has a Lebesgue density π_{prior} and the posterior density π_* exists, given as

$$\pi_*(y) \propto \exp(-\Phi(y)) \tag{2}$$

with log-likelihood potential $L(y) := 1/2|\tilde{\Delta} - \mathcal{G}(y)|^2_\Gamma$ and a potential Φ of the form

$$\Phi(y) := L(y) - \log \pi_{\text{prior}}(y), \tag{3}$$

2 Aims and Methodology

In this work we are concerned with the problem of sampling from the posterior distribution given by (2) using interacting particle methods based on Langevin dynamics. While non-interacting particle systems exhibit slow convergence in time, their extensions to interacting

particle system such as affine invariant Langevin Dynamics [2] and the ensemble Kalman samplers [1] have demonstrated a superior convergence speed. However, such state-of-the-art methods still require a vast number of forward calls to solve the underlying model. Furthermore, convergence to more involved posteriors such as multimodal distributions may become arbitrarily slow or cannot be guaranteed at all. To address these drawbacks, we propose to extend existing methods by the following two strategies.

The first concept is *ensemble enrichment*. It allows to work with ensembles of small batch sizes for large parts of the process, utilizing the contained information to build larger ensembles with the desired distribution at a later time. This substantially reduces the number of necessary calls of the forward model $\mathcal{G}(\cdot)$.

The second concept is based on the notion of *homotopy*. Here, instead of directly working with a particle system based on the posterior, we utilize intermediate measures obtained from interpolation between a simple auxiliary measure and the posterior through a map $\mathcal{H}$ Such a preconditioning of the particle ensemble potentially increases the convergence speed over time significantly, especially for multimodal distributions.

Then our investigation is concerned with an interacting particle system of the form

$$\mathrm{d}y_t^{(i)} = b_{\mathcal{H}}(t, Y_t)\mathrm{d}t + \Gamma(Y_t)\mathrm{d}W_t^{(i)}, \quad i = 1 \ldots, B \in \mathbb{N} \tag{4}$$

with a designed time-inhomogeneous drift term $b_{\mathcal{H}}$, defined upon the homotopy map $\mathcal{H}$ and a varying number of particles B.

We discuss advantages and disadvantages of different enrichment schemes. Moreover we analyse the convergence of the proposed method in expected 2-Wasserstein distance and underline the efficiency of the method with various numerical examples, including non-linear forward maps $\mathcal{G}$ and multi-modal target distributions.

3 Acknowledgements

RG acknowledges financial support within Math+ project *EF1-25: Wasserstein Gradient Flows for Generalised Transport in Bayesian Inversion.*

References

[1] A. Garbuno-Inigo, F. Hoffmann, W. Li, and A. M. Stuart. Interacting Langevin diffusions: Gradient structure and ensemble Kalman sampler. *SIAM Journal on Applied Dynamical Systems*, 19(1):412–441, 2020.

[2] A. Garbuno-Inigo, N. Nusken, and S. Reich. Affine invariant interacting Langevin dynamics for Bayesian inference. *SIAM Journal on Applied Dynamical Systems*, 19(3):1633–1658, 2020.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Dimension-independent Markov chain Monte Carlo on the sphere

Han Cheng Lie [*], **Daniel Rudolf**[**], **Björn Sprungk**[†], **and Tim J. Sullivan**[‡]

[*] Institut für Mathematik, Universität Potsdam
Potsdam, Germany
e-mail: hanlie@uni-potsdam.de

[**] Universität Passau
Passau, Germany
e-mail: daniel.rudolf@uni-passau.de

[†] Faculty of Mathematics and Computer Science, TU Bergakademie Freiberg
Freiberg, Germany
e-mail: bjoern.sprungk@math.tu-freiberg.de

[‡] Mathematics Institute and School of Engineering, University of Warwick
Coventry, United Kingdom
e-mail: t.j.sullivan@warwick.ac.uk

Abstract: In many applications the parameter to be inferred does not belong to a linear space but rather a nonlinear manifold such as the sphere, e.g., in level-set inversion, density estimation or shape analysis. We consider Bayesian inference for such parameters and focus on angular central Gaussian priors. These priors model antipodally-symmetric directional data and are easily defined in Hilbert spaces. We then propose novel efficient Markov chain Monte Carlo methods for approximate sampling of posteriors resulting from conditioning these priors on noisy data. Our approach relies on lifting the sampling problem to the ambient Hilbert space and exploit existing dimension-independent sampling methods in linear spaces. By a push-forward Markov kernel construction we then obtain Markov chains on the sphere, which inherit reversibility and spectral gap properties from the samplers in the ambient linear spaces. In particular, our proposed algorithms have a dimension-independent efficiency which is verified in numerical experiments.

Keywords: Bayesian inverse problems, Sampling menthods, manifolds,

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Response-surface-based Bayesian inversion for engineering applications

Chiara Piazzola* **and Lorenzo Tamellini†**

* Department of Mathematics, Technical University of Munich
Munich, Germany
e-mail: chiara.piazzola@tum.de

† Institute for Applied Mathematics and Information Technologies "E. Magenes",
National Research Council (IMATI-CNR)
Pavia, Italy
e-mail: tamellini@imati.cnr.it

Abstract: In this work we take a look at the methods and challenges of the inverse uncertainty quantification analysis of complex engineering systems. In particular, we illustrate how to employ a Bayesian approach to take advantage of information coming from experimental data to estimate the probability density function of the model parameters. The methodology relies on many calls to the computational model for different configurations of the parameters and evaluates the plausibility of each of them with respect to the available data. Since the simulation of such complex systems is usually computationally very expensive, we make use of response surfaces (also known as surrogate models) that approximate the parametric response of the system and have the advantage of being cheaper to evaluate than the full model. Besides, we get a glimpse of the parameter identifiability analysis, i.e. the "theoretical" discussion on whether model parameters can actually be estimated depending on the type of data available. We consider a simple dynamical system, an additive manufacturing process, and a land subsidence problem to exemplify the discussion.

Keywords: Uncertainty quantification, Bayesian inversion, response surfaces, parameter identification

1 Extended abstract

Complex engineering systems are usually described by mathematical models that are often high-dimensional. The high-dimensionality is due to the need of including several parameters to exhaustively describe the physical behavior and the geometry of the system. Therefore, the simulation of such systems results to be computationally very expensive, often demanding for high performance computing architectures. Besides, such parameters are generally modeled by random variables, to take into account e.g. their inherent variability, imperfect knowledge, or modeling inadequacy, ... Hence, exploring the parameter space, and, especially the parametric response of the system can be very costly, e.g. in case of optimization and Uncertainty Quantification (UQ) analyses.

In this work we focus on UQ analysis, that has been proven to be a suitable tool to assess the impact of parameters uncertainties on the quantity of interest of the system. Specifically, we investigate the so-called inverse UQ analysis, and in particular, the Bayesian approach, that aims at reducing the uncertainty assigned a-priori to the model parameters, estimating the plausibility of different possible parameter values given a set of experimental data. Note that inverse UQ analysis can be seen as closely related to parameter calibration, but – instead

of providing a specific value for the calibrated parameters – it returns a "data-informed" parameter distribution, usually known as posterior distribution.

To reduce the computational burden of the procedure, a possible way out is to build an approximation of the parametric response of the system, often called response surface (or surrogate model), i.e. an approximation of the parametric function that maps the input parameters to quantities of interest of the system. Querying many times such response surface for different parameter configurations is expected to be considerably cheaper than querying the full model. Crucially, such approximations need to be constructed in a wise way making use of a limited number of full model evaluations. Some possibilities that have been explored in the literature are interpolants, least-squares approximations, neural networks, ... Furthermore, multi-fidelity response surfaces can also be used, that are obtained combining evaluations of the full model with different levels of accuracy (i.e. different fidelities), ideally many low-fidelity solutions (which are cheap to evaluate) and few high-fidelity ones (which are instead more expensive) to balance the accuracy and the computational cost required to build them.

Further, we discuss on the well-posedness of the inverse problem, i.e. whether there exist a certain set of parameters that generates the available data. This is the so-called parameter identifiability analysis, and it is a two-step process. At first, the analysis focuses on the ideal case of having perfect noiseless data. By means of analytic tools one can reveal whether all the model parameters can be recovered from such data and possibly uncover correlations between them that could preclude their estimation. Second, the realistic case is considered: parameter identifiability is studied by means of numerical tools in the case of synthetic noisy data. The parameter identifiability analysis should be understood as a preliminary step to the Bayesian inversion: it guarantees the reliability of the estimation of the distribution of the parameters and, consequently, of the simulations.

We illustrate the workflow by means of a simple dynamical system [1] and discuss its application to an additive manifacturing process [2] and a land subsidence problem.

2 Acknowledgements

The authors have been supported by the PRIN 2017 project 201752HKH8 Numerical Analysis for Full and Reduced Order Methods for the effcient and accurate solution of complex systems governed by Partial Differential Equations (NA-FROM-PDEs)".

References

[1] C. Piazzola, L. Tamellini, R. Tempone. A note on tools for prediction under uncertainty and identifiability of SIR-like dynamical systems for epidemiology. Math. Biosci., 332, 108514, 2021.

[2] M. Chiappetta, C. Piazzola, M. Carraturo, L. Tamellini, A. Reali, and F. Auricchio. Inverse and forward sparse-grids-based uncertainty quantification analysis of laser-based powder bed fusion of metals. Submitted, 2022. arXiv:2210.06839

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Explicable least-squares Petrov-Galerkin nonlinear manifold method with hyper-reduction

Romor Francesco*, Stabile Giovanni† Rozza Gianluigi†

* Department of Mathematics
International School for Advanced Studies (SISSA)
Trieste, Italy
e-mail: francesco.romor@sissa.it

† Department of Mathematics
International School for Advanced Studies (SISSA)
Trieste, Italy
e-mail: giovanni.stabile@sissa.it
e-mail: gianluigi.rozza@sissa.it

Abstract: Non-affine parametric dependencies, nonlinearities and advection-dominated regimes of the model of interest can result in a slow Kolmogorov n-width decay, which precludes the realization of efficient reduced-order models based on linear subspace approximations. Among the possible solutions, there are purely data-driven methods that leverage autoencoders and their variants to learn a latent representation of the dynamical system, and then evolve it in time with another architecture. Despite their success in many applications where standard linear techniques fail, more has to be done to increase the interpretability of the results, especially outside the training range and not in regimes characterized by an abundance of data. Not to mention that none of the knowledge on the physics of the model is exploited explicitly during the predictive phase. In order to overcome these weaknesses, we implement the non-linear manifold method introduced by Carlberg et al [2] with hyper-reduction achieved through reduced over-collocation and teacher-student training of a reduced decoder, or other variants. We test the methodology on a 2d non-linear conservation law, a 2d shallow water, and a 2d compressible flow over an airfoil models, and compare the results obtained with a purely data-driven method for which the dynamics is evolved in time with a long-short term memory network (LSTM).

Keywords: nonlinear model order reduction, scientific machine learning, slow-decaying Kolmogorov n-width

References

[1] Romor, Francesco, Giovanni Stabile, and Gianluigi Rozza. "Non-linear manifold ROM with Convolutional Autoencoders and Reduced Over-Collocation method." arXiv preprint arXiv:2203.00360 (2022).

[2] Lee, Kookjin, and Kevin T. Carlberg. "Model reduction of dynamical systems on nonlinear manifolds using deep convolutional autoencoders." Journal of Computational Physics 404 (2020): 108973.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Sparse Data-Driven Quadrature Rules via ℓ^p-Quasi-Norm Minimization

Manucci Mattia*, Jose Vicente Aguado† and Borzacchiello Domenico†

* Division of Mathematics
Gran Sasso Science Institute
L'Aquila, Italy
e-mail: mattia.manucci@gssi.it

† Institut de Calcul Intensif
École Centrale de Nantes
Nantes, France
e-mail: jose.aguado-lopez@ec-nantes.fr, domenico.borzacchiello@ec-nantes.fr

Abstract: We present the focal underdetermined system solver as numerical tool to recover sparse empirical quadrature rules for parametrized integrals from existing data. This algorithm, originally proposed for image and signal reconstruction, relies on an approximated ℓ^p-quasi-norm minimization. Compared to ℓ^1-norm minimization, the choice of $0 < p < 1$ provides a natural framework to accommodate usual constraints which quadrature rules must fulfil. We also extend an a priori error estimate available for the ℓ^1-norm formulation by considering the error resulting from data compression. Finally, we present numerical examples to investigate the numerical performance of our method and compare our results to both ℓ^1-norm minimization and nonnegative least squares method.

Keywords: Sparse Quadrature Rules, FOCUSS Algorithm, Linear Programming, Parametrized Integrals, Parametrized PDEs, Hyper-Reduction

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Non-intrusive data-driven reduced-order modeling for time-dependent parametrized problems

Junming Duan* **and Jan S. Hesthaven†**

* Chair of Computational Mathematics and Simulation Science
École Polytechnique Fédérale de Lausanne
Lausanne, Switzerland
e-mail: junming.duan@epfl.ch

† Chair of Computational Mathematics and Simulation Science
École Polytechnique Fédérale de Lausanne
Lausanne, Switzerland
e-mail: jan.hesthaven@epfl.ch

Abstract: The reduced-order model is efficient and reliable in the context of multi-query or real-time problems. However, the linear reduced space is not efficient for time-dependent nonlinear problems, especially for transport-dominated problems. And the non-linearity usually needs to be addressed by the hyper-reduction technique such as DEIM. This talk will present a new non-intrusive data-driven reduced-order modeling approach for time-dependent parametrized problems. During the offline stage, the convolutional autoencoder consisting of encoder and decoder is trained to perform the dimensionality reduction. The encoder compresses the full-order solution snapshots to a nonlinear latent space. The decoder part can be used to recover the full-order solution from the latent space. To deal with the time-dependent problems, the high-order dynamic mode decomposition (HODMD) is utilized to model the trajectories in the latent space for each parameter. At the online stage, the HODMD are first utilized to obtain the latent variables at a new instant, then some interpolation techniques are adopted to get the latent variables at a new parameter, finally the full-order solution is recovered by the decoder. Some numerical tests are conducted to show that our approach can be used to predict the unseen full-order solution at new instants and parameters fast and accurately.

Keywords: Reduced-order modeling, convolutional autoencoder, dynamic mode decomposition, parametrized problem, time-dependent problem, nonlinear problem

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Incorporating geometrical domain information into Gaussian Processes and Neural Networks for modelling physical fields

Mariella Kast[*], **Mengwu Guo**[†], **Jan Hesthaven**[*]

[*]École Polytechnique Fédérale de Lausanne (EPFL), Switzerland
e-mail: mariella.kast@epfl.ch

[†] University of Twente, Netherlands
e-mail: m.guo@utwente.nl

Abstract: We explore a new method to incorporate knowledge about boundary conditions (BCs) and domain geometry into Gaussian Processes (GPs) and by extension into physics informed neural-networks (PINNs). Both of these machine learning methods have become popular surrogates for partial differential equations (PDEs) that model physical fields. For a lot of engineering applications, a limited number of measurements as training data remains a critical challenge in achieving the required accuracy of the surrogate model. We show how the eigenfunctions of the Laplace operator can be used to to enforce Dirichlet and Neumann boundary conditions (BCs) exactly for a predicted surrogate solution field. At the same time this can encode geometrical information about domains with complicated shapes, e.g. with holes or truss structures, which facilitates learning. Our numerical experiments show that our approach can reduce the number of required samples/training time and increase accuracy of the predicted solution compared to standard GPs and PINNs. We further discuss the practical limitations and theoretical connections between the two methods on simple engineering examples.

Keywords: Surrogate modelling, enforcing boundary conditions, complex gemetrical domains

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Graph convolutional autoencoder architecture for model order reduction of parametrized PDEs

Federico Pichi*, Beatriz Moya† and Jan S. Hesthaven*

* Chair of Computational Mathematics and Simulation Science
École Polytechnique Fédérale de Lausanne
1015 Lausanne, Switzerland
e-mail: federico.pichi@epfl.ch, jan.hesthaven@epfl.ch

† Aragon Institute in Engineering Research (I3A)
University of Zaragoza
50018 Zaragoza, Spain
e-mail: beam@unizar.es

Abstract: In this work, we develop a nonlinear model order reduction technique exploiting an Autoencoder architecture based on Graph Convolutional Networks. We are interested in obtaining fast evaluations of parametrized partial differential equations (PDEs) in a many-query context, where reduced order models (ROMs) are crucial to alleviate the computational cost associated. Despite their robustness, standard ROM techniques, such as Proper Orthogonal Decomposition (POD), struggle when dealing with non-affine or nonlinear parametrized problems. Deep learning techniques allow for non-intrusive analysis, i.e. the autoencoder architecture generalizes the POD approach. We present a data-driven and nonlinear reduction technique exploiting Graph Neural Networks, as they naturally represent fields on unstructured meshes, embedded in a convolutional autoencoder. We applied the methodology to several multi-parametrized test cases, featuring nonlinearities, geometrical parametrization, slow Kolmogorov-decay and bifurcations.

Keywords: Graph neural networks, convolutional autoencoders, model reduction, parametrized PDEs

1 Introduction

When dealing with the numerical approximation of parametrized PDEs, the exploitation of high-fidelity techniques is usually unfeasible due to the large number of degrees of freedom involved. This becomes even more challenging if one needs multiple evaluations of the solution field in a fast and reliable way. Reduced Order Models (ROMs) have been thoroughly investigated to pursue this goal [5], aiming at decoupling the computation in offline and online phases, during the latter of which one only solves a low-dimensional system. Consisting in a linear expansion over the basis of the reduced space, the standard ROM approach looses all the efficiency when non-affine and nonlinear terms are present in the model.

2 Graph convolutional autoencoder architecture (GCA-ROM)

During the last decade, several approaches exploiting machine learning paradigms have been analyzed from the reduced order modelling community. Non-intrusive linear techniques, such as POD-NN [1, 2], allow obtaining efficient computations, but they still depend on the POD accuracy. Deep-learning approaches based on convolutional autoencoders are simultaneously

generalizing the POD compression procedure extracting relevant information from data, and allowing for fast non-linear reconstruction of the solution fields [3]. However, these techniques are not consistent in the case of unstructured or changing meshes.

Introducing the GCA-ROM approach [4], we provide a machine learning framework to deal with models defined on unstructured grids, capturing their geometric features through a combination of Graph Neural Networks and Convolutional Autoencoders. The architecture (see Figure 1) can cope with parametrized scalar/vector and linear/nonlinear PDEs, possibly exploiting pooling operations to down-sample large meshes. Our approach is characterized by spatial convolutions, defined on neighbourhoods of nodes through message passing and aggregation procedures. We considered several physical and geometrical multi-parametrized models, such as Poisson, Graetz and Navier-Stokes. Moreover, we analyzed its performance for bifurcating and advection-dominated problems, for which classical ROMs are not suited.

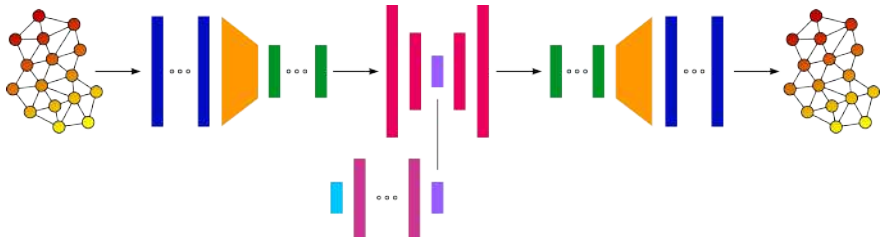


Figure 1: GCA-ROM network structure for the offline phase.

3 Conclusions

We developed a novel non-intrusive reduced-order architecture based on Graph Convolutional Autoencoder. Among the advantages, we highlight the high-generalizability in the low-data regime and the great speedup. Several investigations will be conducted exploiting this architecture: time-dependent PDEs, and different convolution/pooling operators.

References

[1] Hesthaven, J. S. and Ubbiali, S. Non-intrusive reduced order modeling of nonlinear problems using neural networks. Journal of Comp. Physics, 363, pp. 55-78, 2018.

[2] Pichi, F. et al. An artificial neural network approach to bifurcating phenomena in computational fluid dynamics. arXiv:2109.10765, 2021.

[3] Fresca, S., Dedé, L. and Manzoni, A. A Comprehensive Deep Learning-Based Approach to Reduced Order Modeling of Nonlinear Time-Dependent Parametrized PDEs. Journal of Scientific Computing, 87(2), p. 61, 2021.

[4] Pichi, F., Moya, B. and Hesthaven, J. S. A graph convolutional autoencoder approach to model order reduction for parametrized PDEs. Unpublished results, 2023.

[5] Hesthaven, J. S., Rozza, G. and Stamm, B. Certified Reduced Basis Methods for Parametrized Partial Differential Equations, 2016. Cham: Springer Int. Publishing.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Physics informed Generative Adversarial Networks for interactive structural shell design

Moya, Beatriz*, Chinesta, Francisco† and Cueto, Elías*

* Aragon Institute in Engineering Research (I3A)
School of Engineering and Architecture, University of Zaragoza
Zaragoza, Spain
e-mail: {beam, ecueto}@unizar.es

† ESI Group Chair at the PIMM Lab
Arts et Mètiers Institute of Technology
Paris, France
e-mail: francisco.chinesta@ensam.eu

Abstract: Modern architectural modeling software tends to focus on geometry rather than performance. Shape, forces, and materials seem to have irreconcilable differences. Shell structures emerge as an efficient construction solution to cover large spans with minimum material use. However, their design requires guaranteed bending-free behavior. Although catenary or hyperbolic paraboloids are known to provide the desired axial balance in 2D compositions, the design of 3D shells is not solved.

There is a resurgence of interest in techniques that merge geometry and forces to choose the best design through real-time interaction between the two aspects. This is the case of graphic statics, which consists of a graphical force calculation technique for discretized structures working exclusively under axial loads. Recently developed computational tools exist based on this theory [1][2]. The apriori assumption of axial forces is crucial for the design of shell structures.

In the spirit of topology tools, artificial intelligence can be a framework to learn to generate new shapes under certain constraints [3]. However, only by employing a physical criterion can good performance be guaranteed. We propose the use of Generative Adversarial Networks (GAN) guided by physical constraints [4]. GANs are composed of two networks. The first one is in charge of generating new designs by learning the manifold of the geometries. The second network will learn to estimate the axial and shear energy of the shells, and the shell rate to penalize shapes that do not meet a shear-free description, leading to the improvement of the first network.

This technique is tested in a variety of 2D and 3D scenarios and lays the groundwork for training the network for complex architectures, such as for the design of new materials at the microscopic scale.

Keywords: Shell structures, Physics-informed machine learning, Generative Adversarial Networks

References

[1] Hablicsek, M., Akbarzadeh, M., & Guo, Y. (2019). Algebraic 3D graphic statics: Reciprocal constructions. Computer-Aided Design, 108, 30-41.

[2] Fivet, C., & Zastavni, D. (2013). Constraint-based graphic statics: new paradigms of computer-aided structural equilibrium design. Journal of the International Association for shell and spatial structures, 54(4), 271-280.

[3] Bastek, J. H., & Kochmann, D. M. (2023). Physics-Informed Neural Networks for shell structures. European Journal of Mechanics-A/Solids, 97, 104849.

[4] Goodfellow, I., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., ... & Bengio, Y. (2020). Generative adversarial networks. Communications of the ACM, 63(11), 139-144.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Physics-augmented neural networks meet hyperelasticity: A guide how to enforce general physical requirements

Lennart Linden[*,†], **Karl Kalina**[†], **Jörg Brummund**[†] **and Markus Kästner**[†]

[†] Institute of Solid Mechanics
Chair of Computational and Experimental Solid Mechanics
01062 Dresden, Germany

[*] e-mail: lennart.linden@tu-dresden.de

Abstract: The long-standing challenge of fulfilling the mechanical principles for hyperelastic constitutive models all at once, which have been widely debated over the last few decades, could be seen as "the main open problem of the theory of material behavior" [3]. In this contribution, a hyperelastic constitutive model based on physics-augmented neural networks (PANNs) is presented which fulfills all common physical requirements by construction, and in particular, is applicable for compressible material behavior. This model combines the theory of hyperelasticity developed in the last decades with the up-to-date techniques of machine learning, by formulating a hyperelastic potential as a input-convex neural network (NN). This potential fulfills conditions such as compatibility with the balance of angular momentum, objectivity, material symmetry, polyconvexity, and thermodynamic consistency [1, 2]. Analytical growth terms and normalization terms, formulated for both isotropic and transversely isotropic material behavior, are used to ensure a physically sensible stress behavior of the model and to guarantee that the undeformed state is stress free and with zero energy. The non-negativity of the hyperelastic potential is numerically verified by sampling the space of admissible deformations states. Finally, the applicability of the model is demonstrated by calibrating it on data generated with analytical potentials and by applying it to finite element (FE) simulations. Its extrapolation capability is compared to models with reduced physical background, showing excellent and physically meaningful predictions with the proposed PANN.

Keywords: Hyperelasticity, Physics-augmented neural networks, Physical constraints, Stress normalization

References

[1] Kalina, K. A., Linden, L., Brummund, J. and Kästner, M., FEANN - An efficient data-driven multiscale approach based on physics-constrained neural networks and automated data mining, Comput. Mech. (accepted 2022).

[2] Kalina, K. A., Linden, L., Brummund, J., Metsch, P. and Kästner, M., Automated constitutive modeling of isotropic hyperelasticity based on artificial neural networks, Comput. Mech. 69 (2022).

[3] Truesdell, C. and Noll, W., The Non-Linear Field Theories of Mechanics. 3rd ed. Springer Berlin Heidelberg, 2004.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Performing sensitivity analysis with physics-informed neural networks

Hanna John M.[*†], Aguado José V. [*], Comas-Cardona Sebastien[*], Askri Ramzi[†] and Borzacchiello Domenico[*]

[*] CNRS, GeM, UMR 6183
Nantes Université, Ecole Centrale Nantes
Nantes, France

[†] Nantes Université, IRT Jules Verne
Bouguenais, France

Abstract: Sensitivity analysis studies the effect of small changes in input parameters on output quantities. This work presents a way to perform sensitivity analysis using the paradigm of physics-informed neural networks (PINN). We train PINN to minimize not only the residual of the partial differential equation (PDE), but also the derivative of the residual with respect to the input parameter of interest (POI), while respecting the given initial and boundary conditions. After training, we obtain a good solution within a small neighborhood around the nominal value of the input POI which allows to easily obtain the sensitivity (derivative of the output with respect to the POI). The computation time of the method grows linearly as the number of POIs studied increases which is an advantage. Two examples are presented to show the effectiveness of the technique. The first is a 2D Poisson's problem with multiple POIs. The second is a two-phase flow in porous media problem solved with the Volume of Fluids technique; this problem is chosen to show the method's ability to solve problems including discontinuities.

Keywords: Physics-informed neural networks, sensitivity analysis, two-phase flow in porous media.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Scalar Field Prediction on Structural Analysis using Graph Neural Networks

Ribeiro, B.A.[*12†], Ribeiro, J.A.[*234†], Ahmed, F.[3], Tavares, S.M.O[5], Penedones, H.[2], Sarmento, L.[2] and Belinha, J.[6]

[*] **These two authors contributed equally to this work**
[†] **B.M.AlvesRibeiro@tudelft.nl & jpar@mit.edu**

[1] Department of Materials Science and Engineering. Delft University of Technology. Delft, Netherlands
[2] Inductiva Research Labs. Porto and Lisbon, Portugal
[3] Department of Mechanical Engineering. Massachusetts Institute of Technology. Cambridge, MA
[4] Department of Mechanical Engineering. Faculty of Engineering, University of Porto. Porto, Portugal
[5] Department of Mechanical Engineering, Centre for Mechanical Technology & Automation. University of Aveiro. Aveiro, Portugal
[6] Department of Mechanical Engineering. School of Engineering, Polytechnic of Porto. Porto, Portugal

Abstract: In designing complex structures subject to multi-effects, numerical simulations are essential to obtain the best design option. However, time-consuming multi-physics simulations are a significant challenge that limits the exploration of the design space. To mitigate this limitation, a deep learning model is proposed for predicting scalar fields with very low latency, such as the von Mises stress field, whose values are typically used as selection criteria. The proposed method is based on Graph Neural Networks (GNNs). We show that our model can be robust enough to generalise to different geometries. The data used to train this model comes from a dataset, designed and filled for this type of cases. The case under study is a rectangular plate with six circular holes loaded biaxially. One thousand cases were used, containing variations on the geometry of the holes. An average R-square of 0.9 was obtained for the training data, and 0.6 and 0.5 for the model's interpolation and extrapolation, respectively. In future work, this model will be trained for a larger dataset, aiming to increase its robustness and evaluate its generalisation for different boundary conditions.

Keywords: Graph Neural Networks, Structural Analysis, Computational Design, Machine Learning

1. Introduction

Several machine learning techniques have emerged with the potential to create disruptive methods, improving the scalar field prediction [1]. Artificial Neural Networks (ANNs) [2], Convolution Neural Networks (CNNs) [3], Physical Neural Networks (PINNs) [4], and Graph Neural Networks (GNNs) [5], are examples of tools that can be exploited on the computational mechanics field, aiming to develop a new generation of filed prediction. The general approach is to train a model capable of quickly predicting, to a given degree of approximation, the relevant mechanical response of the system under design and use that prediction to guide the exploration in the design space. However, these learning techniques could also be employed to create digital-twins and to improve the pre-processing and post-processing, for instance, creating optimised meshes of complex parts, assisting problem solving.

In recent years, the popularity of GNNs has increased significantly in several fields where data can be naturally represented as a graph. It is a powerful and practical tool in machine learning tasks [6]. However, like any ML technique, model generation is one of the problems. The main goal is to build a model capable of generalising to different conditions, such as geometry, boundary, and loading conditions, correctly predicting scalar fields. This study will focus primarily on the generalisation of geometry.

2. Methodology

This research aims to predict the von Mises stress field using a GNN model. Therefore, it will be necessary to use a graph dataset to train and evaluate the model to accomplish the primary goal. For this purpose, the SimuStruct dataset, a previously developed dataset, was used.

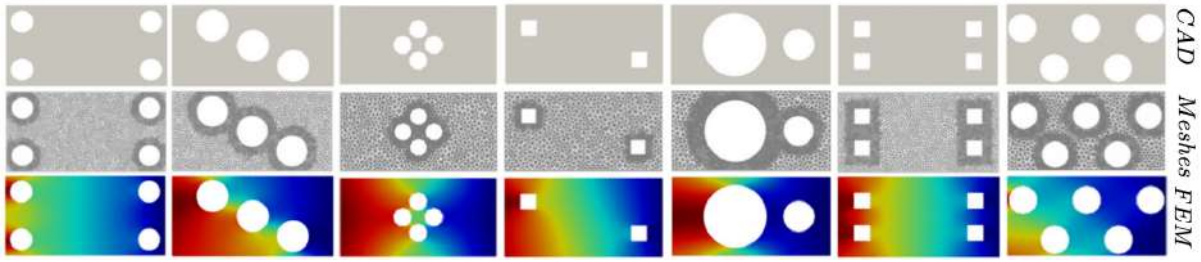


Figure 1. SimuStruc dataset: A dataset that contains the CAD model, the meshes, and the structural simulations (FEM) for different levels of refinement, different properties for a linear and elastic material, and different boundary and loading conditions.

The dataset contains 1000 cases of rectangular plates with six circular holes loaded biaxially. From one case to another, only the position and size of the circular holes vary; all other properties are fixed. The model has the Encoder-Processor-Decoder structure with 30 message-passing layers. The nodal features are the Signed Distance Field (SDF) value, and one-hot identifiers indicate a displacement or load condition. Edges features are the geometric information Δx, Δy, and edge length $||x||$. One of the results obtained by the GNN is presented and compared with the FEM results, see Figure 2.

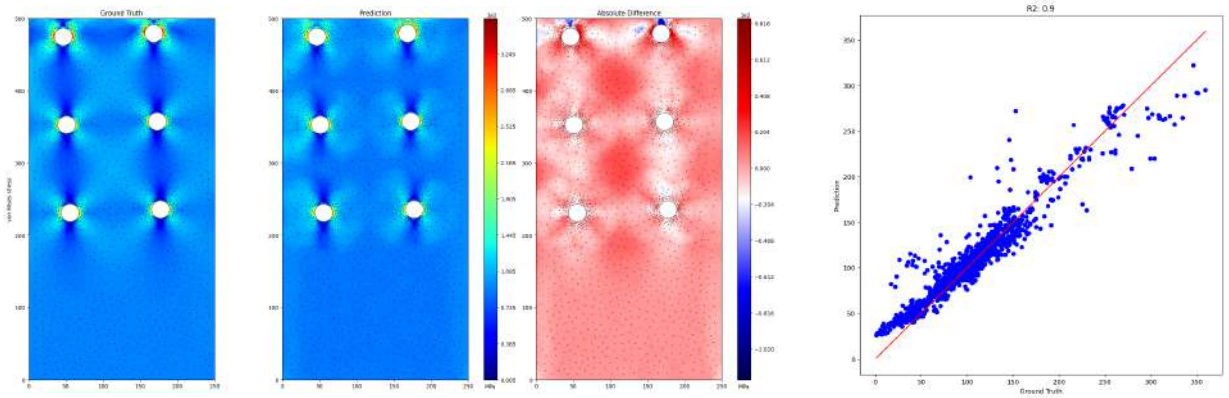


Figure 2. von Mises stress field obtained by the GNN with comparison to FEM through absolute error and R-squared (R2).

3. Conclusions

The developed GNN model showed promising results, with an average R-square for the training of 0.89. However, when evaluating the interpolation and extrapolation of the model, predictions for smaller and larger circular holes, respectively, than those used in training, the model presented an average R-square of 0.6 and 0.5, respectively. It was possible to show the potential of scalar field prediction on structural analysis.

Future work will train the model for a larger dataset to improve the model's generalisation for different geometries. Furthermore, we will study the model's generalisation for different boundary conditions.

References

[1] Yao H, Gao Y, Liu Y. FEA-Net: A physics-guided data-driven model for efficient mechanical response prediction. Computer Methods in Applied Mechanics and Engineering 2020;363(7):112892.

[2] Ribeiro J, Tavares SMO, Parente M. Stress–strain evaluation of structural parts using artificial neural networks. Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications 2021;235(6):1271-1286.

[3] Nie Z, Jiang H, Kara LB. Stress field prediction in cantilevered structures using convolutional neural networks. Journal of Computing and Information Science in Engineering 2020; 20(1):011002.

[4] Haghighat E, Raissi M, Moure A, Gomez H, Juanes R. Computer Methods in Applied Mechanics and Engineering 2021;379:113741.

[5] Pfaff T, Fortunato M, Sanchez-Gonzalez A, Battaglia PW. Learning mesh-based simulation with graph networks. International Conference on Learning Representations 2021.

[6] Zhou J, Cui G, Zhang Z, Yang C, Liu Z, Sun M. Graph Neural Networks: A Review of Methods and Applications. AI Open 2020;1 :57-8.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

SimuStruct: Simulated Structural Plate with Holes Dataset for Machine Learning Application

Ribeiro, B.A.[*12†], Ribeiro, J.A.[*234†], Ahmed, F.[3], Tavares, S.M.O[5], Penedones, H.[2], Sarmento, L.[2] and Belinha, J.[6]

[*] **These two authors contributed equally to this work**
[†] **B.M.AlvesRibeiro@tudelft.nl & jpar@mit.edu**

[1] Department of Materials Science and Engineering. Delft University of Technology. Delft, Netherlands
[2] Inductiva Research Labs. Porto and Lisbon, Portugal
[3] Department of Mechanical Engineering. Massachusetts Institute of Technology. Cambridge, MA
[4] Department of Mechanical Engineering. Faculty of Engineering, University of Porto. Porto, Portugal
[5] Department of Mechanical Engineering, Centre for Mechanical Technology & Automation. University of Aveiro. Aveiro, Portugal
[6] Department of Mechanical Engineering. School of Engineering, Polytechnic of Porto. Porto, Portugal

Abstract: The SimuStruct dataset comprises a 2D version of the classic case of plates with holes since it is a base element found in many different mechanical design applications. The dataset comprises many cases solved using the standard Finite Element Method (FEM) with the open-source software FEniCSx. Note that the entire date is free and available online. Compared to other datasets similar in purpose, SimuStruct is more diversified and realistic because it includes cases for different loading and boundary conditions, different properties for linear and elastic material, and different levels of mesh refinement. In addition, SimuStruct is more flexible, versatile, and scalable because all algorithms and codes are implemented using open-source libraries. The main goal of the SimuStruct dataset is to serve as training and evaluation data for Machine Learning (ML)-based methods in structural analysis and optimal mesh generation and therefore support the development of ML-based optimal mechanical design solutions. We validate SimuStruct by using its data to applied to train and test a multilayer perceptron (MLP) model to predict stress-strain fields. Our goal with publishing SimuStruct is to contribute to the connection of the Mechanical Engineering and ML communities, which will accelerate and exploit research in the computational design field.

Keywords: Plate with Holes, Structural Analysis, Computational Design, Machine Learning, Finite Element Method

1. Introduction

Recent advances in computational tools have shown the potential of automatic generative design techniques, surrogate modelling [1-2], and virtualization of complete mechanical systems [3-4]. The two critical components of this automatic design process are a simulator of the object's mechanical properties and an optimization module that automatically searches the space of design parameters to find the configuration that optimises the final solution under certain design restrictions, such as stress or displacement. Traditionally, linear elastic simulation has been performed using the Finite Element Method (FEM), although it has limitations in accuracy in simulating the mechanical properties of the mechanical components, and it is usually too computationally intensive and relatively slow.

In order to alleviate this limitation, several methods based on ML have been proposed [5-11]. However, there are several challenges when using ML approaches. First, ML approaches may not generalise well, i.e. ML models are often specialised in solving only one type of geometric case, and it needs to be clear how to train a model to operate on more than one family of mechanical cases. Second, systematic evaluation and comparison of ML the various ML approaches proposed is challenging due to the need for a standard set of cases against

which we can evaluate all the models. This work introduces the Simulated Structural Plate with Holes Dataset (SimuStruct) aiming to investigate and develop efficient ML procedures for applied mechanics and to help overcome the previous limitations.

2. Methodology

Figure 1 describes all steps to generate and process the dataset. The number of inputs (geometry, Young modulus and Poisson ratios, loading conditions and boundary conditions) is significant, however they are required for a full dataset definition. Future versions could contemplate material constitutive laws, for a more comprehensive dataset.

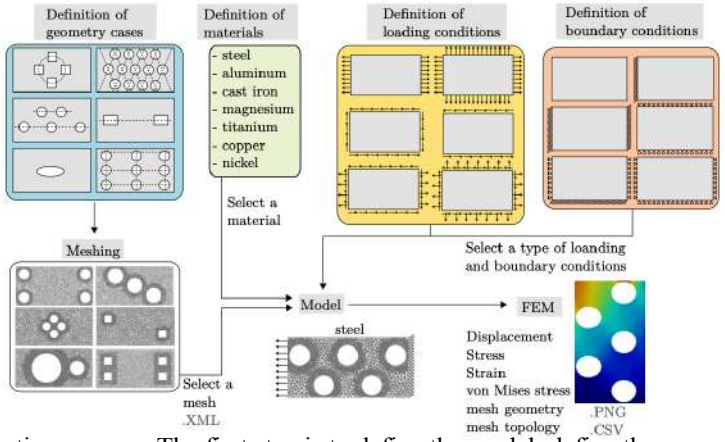


Figure 1. Dataset generation process. The first step is to define the model: define the geometric case and later create the mesh, define the material and loading and boundary conditions; the second step is the FEM-based structural simulation in FEniCSx.

3. Validating the dataset with a baseline ML model

The dataset contains 100 cases of a rectangular plate with six circular holes loaded biaxially. O datset utilizado tem 100 casos geométricos. We aim to predict the von Mises stress field through the MLP model. One of the results obtained by the MLP is presented and compared with the FEM results, see Figure 2.

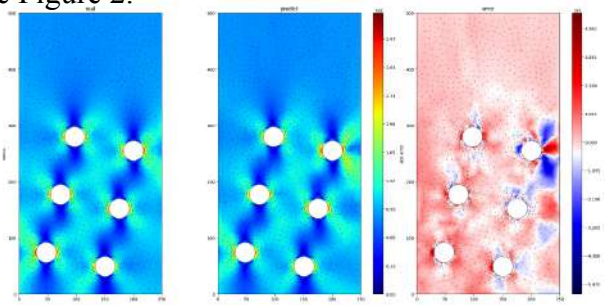


Figure 2. von Mises stress field obtained by the MLP with comparison to FEM through absolute error.

4. Conclusions

SimuStruct is a 2D plate with holes dataset with the geometric model, the meshes, and the structural simulations for different boundary and loading conditions, properties for a linear and elastic material, and varying refinement levels. SimuStruct provides training and evaluation data for ML-based methods, enabling optimal mechanical design solutions. The MLP implementation can correctly predict the von Mises Stress for a given plate with six circular holes and any point on the plate. This application enhances the potential of SimuStruct to train and test ML models in structural mechanics.

References

[1] Yoo S, Lee S, Kim S, Hwang K, Park J, Kang N. Integrating deep learning into CAD/CAE system: generative design and evaluation of 3D conceptual wheel. Structural and Multidisciplinary Optimization 2021;64:2725-2747.

[2] Alderton M. Driving a Lighter, More Efficient Future of Automotive-Part Design at GM. https://redshift.autodesk.com/automotive-design/ (2018); [Accessed: 15-September-2021].

[3] Airbus. Pioneering bionic 3D printing. https://www.airbus.com/newsroom/news/en/2016/03/Pioneering-bionic-3D-printing.html (2016); [Accessed: 21-September-2021].

[4] Alderton M. Reving Up for a Manufacturing Revolution With Hack Rod. https://redshift.autodesk.com/hack-rod/ (2016); [Accessed: 20-September-2021].

[6] Ribeiro J, Tavares SMO, Parente M. Stress–strain evaluation of structural parts using artificial neural networks. Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications 2021;235(6):1271-1286.

[7] Ribeiro J, Gomes L, Tavares SMO. Artificial Neural Networks Applied in Mechanical Structural Design. Journal of Computation and Artificial Intelligence in Mechanics and Biomechanics 2021;1:11-21.

[8] Haghighat E, Raissi M, Moure A, Gomez H, Juanes R. Computer Methods in Applied Mechanics and Engineering 2021;379:113741.

[9] Chen W, Ahmed F. PaDGAN: Learning to Generate High-Quality Novel Designs. Journal of Mechanical Design 2021;143(3):031703.

[10] Nobari AH, Rashad MF, Ahmed F. Creative-gan: Editing generative adversarial networks for creative design synthesis. International Design Engineering Technical Conferences and Computers and Information in Engineering Conference 2021;3A.

[11] Nobari AH, Chen W, Ahmed F. Range-gan: Range-constrained generative adversarial network for conditioned design synthesis. Journal of Mechanical Design 2021;144(2): 021708.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Machine Learning for Discovery and Solution of Partial Differential Equations

Pin ZHANG

Royal Society-Newton International Fellow, Department of Engineering, University of Cambridge, Cambridge, United Kindom
e-mail: dr.pin.zhang@gmail.com

Zhen-Yu YIN
Professor, Department of Civil and Environmental Engineering, The Hong Kong Polytechnic University, Hong Kong, China
e-mail: zhenyu.yin@polyu.edu.hk

Brian SHEIL
Laing O'Rourke Associate Professor, Department of Engineering, University of Cambridge, Cambridge, United Kingdom
e-mail: bbs24@cam.ac.uk

Abstract: Identifying governing equations from data and solving them to acquire spatio-temporal responses is desirable, yet highly challenging, for many practical problems. Machine learning (ML) has emerged as an alternative to influence knowledge discovery in complex geotechnical processes. To demonstrate feasibility, this study develops an ML-assisted data-driven approach to automatically recover Terzaghi's consolidation theory from measured data and obtain the corresponding solutions. This process incorporates several algorithms including sparse regression and prior information based neural network (PiNet), transformed weak-form partial differential equations (PDEs) (to reduce sensitivity to noisy measurement), and Monte Carlo dropout to achieve a measure of prediction uncertainty. The results indicate that consolidation PDEs can be accurately extracted using the proposed approach which is also shown to be robust to noisy measurements. PDEs solved by PiNet are also shown to provide excellent agreement with actual results thus highlighting its potential for inverse analysis. The proposed approach is generic and provides an auxiliary method to verify heuristic interpretations of data or to directly identify patterns and obtain solutions without the need for expert intervention [1].

Keywords: Consolidation; Neural Networks; Uncertainty; Back analysis

References

[1] Zhang P, Yin Z-Y, Sheil B. A physics-informed data-driven approach for consolidation analysis. Géotechnique. 2022:1-12.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Thermodynamics-based digital twins of granular media

Filippo Masi* **and Ioannis Stefanou†**

* Sydney Centre in Geomechanics and Mining Materials,
School of Civil Engineering,
The University of Sydney.
Sydney, Australia.
e-mail: filippo.masi@sydney.edu.au

† Nantes Université, Ecole Centrale Nantes, CNRS,
Institut de Recherche en Génie Civil et Mécanique (GeM), UMR 6183.
Nantes, France.
e-mail: ioannis.stefanou@ec-nantes.fr

Abstract: We present a thermodynamics-based deep learning framework for building digital twins of granular media. The proposed framework relies on Thermodynamics-based Artificial Neural Networks (TANN, [1,2]) and thus enforces thermodynamics consistent predictions of the material behavior. Material datasets are extracted from realistic, fine-scale simulations of geomaterials, using the Discrete Element Method.

Particular attention is focused on the automatic discovering of thermodynamic admissible sets of state variables from fine-scale information via model order reduction techniques [3] and the laws of thermodynamics. Furthermore, the state variables and their evolution can be employed to track, in a simple way, the evolution of the microstructure and its degrees of freedom.

We demonstrate an application of the methodology in modeling the mechanical behavior of sand and faults. The constructed digital twin is able to predict the material response under complex loading paths and always fulfills the thermodynamic consistency requirements.

Keywords: Thermodynamics-based Artificial Neural Networks, Deep Learning, Discrete Element Method, Asymptotic homogenization.

References

[1] Masi F, Stefanou I, Vannucci P, Maffi-Berthier V. Thermodynamics-based Artificial Neural Networks for constitutive modeling. J Mech Phys Solids 2021;147:104277. doi: 10.1016/j.jmps.2020.104277.

[2] Masi F, Stefanou I. Multiscale modeling of inelastic materials with Thermodynamics-based Artificial Neural Networks (TANN). Comput Methods Appl Mech Eng 2022;398:115190. doi: 10.1016/j.cma.2022.115190.

[3] Masi F, Stefanou I. Evolution TANN and the discovery of the internal variables and evolution equations in solid mechanics. arXiv preprint arXiv:2209.13269. 2022. doi: 10.48550/arXiv.2209.13269.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Reduced order models for time-dependent problems using the Laplace transform

Ricardo Reyes*, Fernando Henríquez and Jan Hesthaven

Chair of Computational Mathematics and Simulation Science (MCSS)
Ecole Polytechnique Fédérale de Lausanne (EPFL)
Lausanne, Switzerland
*e-mail: ricardo.reyes@epfl.ch

Abstract: We propose a new method to incorporate temporal evolution into general reduced-order parametrised models. Instead of following the traditional approach of time step sampling, we use frequency-domain solutions as the data input. In the offline stage, we transfer the problem from the time domain to the frequency domain using the Laplace transform. Then, we sample solutions for a discrete set of frequencies and use the singular valued decomposition to construct a reduced basis. And in the online part, we use the obtained reduced basis in the time-dependent problem, as we would normally do with a basis obtained with any parametric or time-sampled reduced basis method. Although the method can be seen as a proper orthogonal decomposition extended to the frequency domain, there are two important considerations: we have to select appropriate sampling points so all the needed frequencies are captured, and we construct the basis using only the real part of the complex-valued solutions. We present some of the harmonic analysis needed to explain the method and a two simple examples.

Keywords: Time-dependent model reduction, Reduced basis method, H^2 Hardy space, Laplace transform

1 Introduction

Although reduced basis methods are suitable and fully capable surrogate models for general parametric problems, constructing a reduced order model for a time-dependent problem can be challenging. Since the solution may evolve without a clear pattern that we can easily predict, we may need to sample solutions over an extensive time period and at a high frequency in order to be accurate. This can be excessively costly and time-consuming.

Reduced basis methods for parametrised time-dependent problems use a mix of Greedy techniques to select the sample set in the parameter space, and a regular interval sampling in the time-domain [1]. An alternative approach to create a reduced model consists in moving the problem to the frequency domain using the Laplace transform, solving the equivalent reducer order frequency problem and using an inverse Laplace transform to go back to the original time domain [2]. Unfortunately, the computation of the inverse Laplace transform may be too expensive and sometimes unattainable in practice.

Our method starts using the Laplace transform to move the problem to the frequency domain, similar to the work in [3]. Here, we follow a proper orthogonal decomposition extended to the frequency-domain problem with two important considerations: we have to select appropriate sampling points so all the needed frequencies are captured, and we construct the basis using only the real part of the complex-valued solutions. Finally, we can use the generated reduced basis in our original problem.

2 Frequency-based reduced basis method

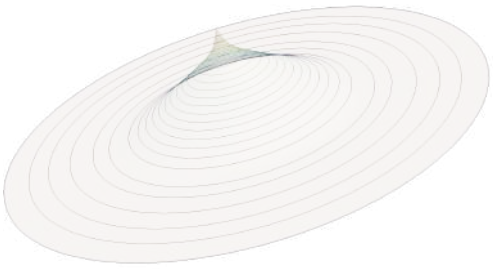
We can describe the method for finding a basis using a discrete set of parameters $\mathbb{P}_h$ and a discrete set of frequencies $\mathbb{F}_h : \{i\cot(\theta),\ \forall\theta \in [-\pi, \pi]\}$

Algorithm 1: Construction of the reduced basis

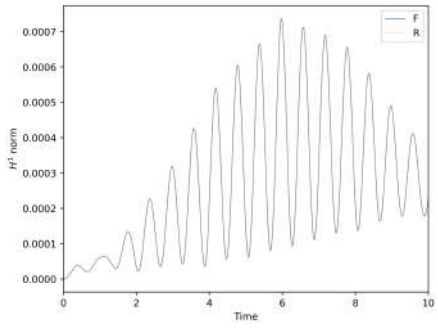
Compute the Laplace $\mathcal{L}$ transform of the original time-dependent problem
for $\boldsymbol{\mu} \in \mathbb{P}_h$ **do**
    for $s \in \mathbb{F}_h$ **do**
        Solve the frequency-domain problem for $\hat{\boldsymbol{u}}_h(\boldsymbol{x}, s; \boldsymbol{\mu})$
Set the real valued data set. $D_h(\mathbb{F}_h, \mathbb{P}_h) = \{\Re\{\hat{\boldsymbol{u}}_h(\boldsymbol{x}, s; \boldsymbol{\mu})\} | s \in \mathbb{F}_h,\ \boldsymbol{\mu} \in \mathbb{P}_h\}$
Construct the basis Φ using a singular value decomposition. $S_h(\mathbb{F}_h, \mathbb{P}_h) = \Phi\Lambda\Psi$

3 Results

We test the new reduced basis method tin the wave equation $u_{tt} + \mu^2\nabla^2 u = \sin(\omega t)e^{\alpha^2(x^2+y^2)}$, for a unit circle domain centered in $(0, 0)$, $\mu = 1.0$, $\omega = 5$ and $\alpha = 200$. We discretize the geometrical space using finite elements, and advance the time evolution using a Newmark-β method. We set the time step $\delta t = 0.01$, the mesh size $h = 0.02$.



(a) Contour plots



(b) H^1-norm

Figure 1: Comparison of the finite element and reduced-order model solutions

References

[1] Jan S Hesthaven, Cecilia Pagliantini, and Gianluigi Rozza. Reduced basis methods for time-dependent problems. *Acta Numerica*, 31:265–345, 2022.

[2] Caterina Bigoni and Jan S. Hesthaven. Simulation-based Anomaly Detection and Damage Localization: an application to Structural Health Monitoring. *Computer Methods in Applied Mechanics and Engineering*, 363:112896, 2020.

[3] Mohamed Aziz Bhouri and Anthony T. Patera. A two-level parameterized model-order reduction approach for time-domain elastodynamics. *Computer Methods in Applied Mechanics and Engineering*, 385:1–21, 2021.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A Thermodynamics-Informed Deep Learning Framework for Turbulent Flow Estimation

Carlos Bermejo-Barbanoj[*], Alberto Badías[†], David González[*], Francisco Chinesta[‡] and Elías Cueto[*]

[*] Aragon Institute in Engineering Research (I3A)
University of Zaragoza, María de Luna s/n, 50018, Zaragoza, Spain
e-mail: {cbbarbanoj, gonzal, ecueto}@unizar.es

[†] Higher Technical School of Industrial Engineering (ETSII)
Polytechnic University Of Madrid, José Gutiérrez Abascal 2, E-28006, Madrid, Spain
e-mail: alberto.badias@upm.es

[‡] ESI chair PIMM Lab Arts et Métiers Institute of Technology
École Nationale Supérieure d'Arts et Métiers, 151 Boulevard d l'Hôpital, 75013, Paris, France
e-mail: francisco.chinesta@ensam.eu

Abstract:

Fluid dynamics is an area that involves very complex phenomena, some of what remains unresolved until today. A complex area inside the fluid dynamics field is aerodynamics. Aerodynamics plays an important role for the vehicle companies, specifically for the designing department. Every year, the research departments of these companies invest lots of resources to improve their products, leading to more efficient designs. For these companies, data-driven methods could lead to a more efficient workflow, helping designers and engineers in the decision making, for instance when choosing between different initial designs.

Nowadays, Computational Fluid Dynamics (CFD) tools provide the user with accurate simulations, allowing companies to save huge amounts of resources when compared with experimental methods. Their main drawback is the amount of CPU time needed to run a single simulation. When complex phenomena, like turbulence, are modelled, the computational cost increases considerably due to the physics underlying them. For that reason, some machine learning approaches have been taken, for example to estimate aerodynamics of a new design when compared with others previously analysed by CFD [1], leading to real-time results with little loss of accuracy.

We introduce a DL approach to estimate some of the most relevant characteristics of the flow around two-dimensional geometries: the pressure (P) and the velocity (U_x and U_y). For this approach, a database of turbulent flows around simple geometries has been generated using OpenFoam, an open-source CFD software. Our approach uses level sets for the codification of the geometry. This coding allows the algorithm to predict out-of-training geometries only using the modified level set. This codification also allows us to use a regular grid, taking advantage of the Convolutional Neural Networks (CNN) architectures. Our method is trained in different phases. First, we use a Variational Autoencoder (VAE) to learn a low dimensional representation of the pressure and velocity fields (P, U_x, U_y) using an encoder-decoder scheme, where both the encoder and the decoder are built using a CNN. Then, we train a separate encoder for the level set and initial velocity of each simulation. This new encoder learns the representation of the first snapshot of each simulation in the low dimensional space previously obtained by the VAE. Finally we train a Structure Preserving Neural Network (SPNN) [3] to calculate and integrate the temporal evolution of the flow in the low dimensional space. The VAE decoder, previously trained, is then used to reconstruct the high dimensional solution. The SPNN applies the GENERIC (*General Equation for Non-Equilibrium Reversible-Irreversible Coupling*) [2] formalism, ensuring that the result obtained is thermodynamically consistent.

Keywords: Turbulence, CFD, Deep Learning, Structure Preserving Neural Network, Thermodynamics

References:

[1] Badías, A., Curtit, S., González, D., Alfaro, I., Chinesta, F. and Cueto, E. An augmented reality platform for interactive aerodynamic design and analysis. Int J Numer Methods Eng; 120:125–138, 2019.

[2] Grmela, M. and Öttinger, H.C. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. Physical Review E, 56(6), p.6620, 1997.

[3] Hernández, Q., Badías, A., González, D., Chinesta, F., Cueto, E. Structure-preserving neural networks. Journal of Computational Physics, vol. 426, p. 109950, 2021.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

AI-enhanced interactive simulators for virtual reality applications

Quercus Hernández*, Alberto Badías†, Francisco Chinesta# and Elías Cueto*

*Aragon Institute of Engineering Research (I3A)
University of Zaragoza
María de Luna s/n, 50018, Zaragoza, Spain
e-mail: {quercus, ecueto}@unizar.es

†Higher Technical School of Industrial Engineering
Polytechnic University of Madrid
José Gutiérrez Abascal 2, E-28006, Madrid, Spain
e-mail: alberto.badias@upm.es

#ESI Chair at the PIMM Lab
Arts et Metiers Institute of Technology
151, Bvd. de l'Hopital, F-75013, Paris, France
e-mail: francisco.chinesta@ensam.eu

Abstract: The imminent impact of immersive technologies in society urges for active research in real-time and interactive physics simulation for virtual worlds to be realistic, thus compliant with the laws of physics. On the one hand, current real-time physic engines rely on severe simplifications of the governing dynamical equations and are limited to simple material models and constitutive phenomena. On the other hand, classical engineering methods for solid and fluid simulations are too expensive to achieve real-time framerates but can be used to generate a rich and consistent database to train a fast AI-accelerated simulator using the recent advances in machine learning procedures.

In this talk, we present an augmented reality set-up to simulate real-time interactive dynamical systems in solid mechanics problems [1]. A stereo camera is used to compute the depth map of an arbitrary scene, place a virtual 3D solid and detect the user hand interaction. When contact is detected, the solid deforms according to a learnt constitutive equation which must be trained in advance. Additional outputs such as stress or displacement fields can also be displayed over the virtual object as a colormap. The rapid performance of the simulation is achieved using a graph-based and structure-preserving deep learning algorithm [2], which ensures the thermodynamical consistency of the predictions by using the GENERIC structure of the problem. Two demos are provided with different geometries and material responses to test the robustness of the method.

Keywords: Artificial Intelligence, Machine Learning, Virtual Reality, Realtime Simulators, GENERIC

References

[1] Hernández, Quercus and Badías, Alberto and Chinesta, Francisco and Cueto, Elías. Thermodynamics-informed neural networks for physically realistic mixed reality. arXiv preprint arXiv:2210.13414, 2022.

[2] Hernández, Quercus and Badías, Alberto and Chinesta, Francisco and Cueto, Elías. Thermodynamics-informed Graph Neural Networks. IEEE Transactions on Artificial Intelligence, DOI 10.1109/TAI.2022.3179681, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A consistent thermodynamic data driven method for dissipative thermomechanics

Portillo David*, Montejo Virginia† and Badías Alberto†

* Department of Mechanical Engineering
ETSII, Universidad Politécnica de Madrid
Madrid, Spain
e-mail: david.portillo@upm.es

† Department of Mechanical Engineering
ETSII, Universidad Politécnica de Madrid
Madrid, Spain

Abstract: Structure preserving integrators have been employed with remarkably success in a broad class of dynamic systems. An important subclass of these systems are the Hamiltonian systems. The general formalism of Hamiltonian problems has enabled the development of general structural preserving methods to different problems, such as molecular dynamics, Euler equations of fluid flow, nonlinear mechanics of solids, etc. However, Hamiltonian systems fail when trying to model dissipative systems, such as thermomechanic problems. For this kind of problems Morrison [1] introduced in the 80's the so called metriplectic systems, which provides a complete framework for the mathematical description of dissipative systems.

We present here a method based on quadratic programing for learning dissipative models from data. For that, we take advantage of the metriplectic structure of the system to preserve the two laws of thermodynamics, i.e. energy conservation and non-decreased entropy. During the talk we will present the basic theory of metriplectic systems for the particular case of thermomecanics and construct a convex problem for extracting the metriplectic structure from data. We will also show numerical examples.

Keywords: Dissipative systems, thermomechanics, structure preserving

References

[1] Morrison PJ. A paradigm for joined Hamiltonian and dissipative systems. Physica D Nonlinear Phenomena 1986, 18.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Towards the simulation of complex systems: Port-Metriplectic Neural Networks

Badías, Alberto*, Hernández, Quercus†, Chinesta, Francisco# and Cueto, Elías†

* Higher Technical School of Industrial Engineering
Polytechnic University of Madrid
José Gutiérrez Abascal 2, E-28006, Madrid, Spain
e-mail: alberto.badias@upm.es

† Aragon Institute of Engineering Research (I3A)
University of Zaragoza
María de Luna s/n, 50018, Zaragoza, Spain
e-mail: {quercus, ecueto}@unizar.es

ESI Chair at the PIMM Lab
Arts et Metiers Institute of Technology
151, Bvd. de l'Hopital, F-75013, Paris, France
e-mail: francisco.chinesta@ensam.eu

Abstract: Currently, the numerical simulation of the behavior of systems is a completely solved task. It is very easy to solve a set of equations applied to a geometry, together with boundary or initial conditions –depending on the problem in question– to be able to simulate the real behavior of the system. However, sometimes the model or equation that governs the behavior of the system is not known. For these cases, it has been verified that the introduction of machine learning techniques based on physically consistent neural networks [1] allows describing the dynamics of the systems without the need for an excessively large set of data. This is due to the introduction of inductive biases that allow optimal use of the symmetries of the problem [2].

However, when it comes to complex problems, the user can tackle the problem in its entirety, or divide the problem into sub-problems. This second option is optimal since it allows the behavior of the sub-systems to be learned separately in order to use them as many times as necessary, as if it were a puzzle, as long as said sub-systems are able to communicate correctly.

In this work we present a method to simulate the behavior of complex systems by learning their dynamics from data, through the local simulation of each subsystem. For this, we use physically consistent artificial neural networks that guarantee compliance with the thermodynamic laws [3].

Keywords: Machine Learning, Complex Systems, GENERIC

References

[1] Hernández, Q., Badías, A., Chinesta, F., and Cueto, E. Thermodynamics-informed neural networks for physically realistic mixed reality. arXiv preprint, arXiv:2210.13414, 2022.

[2] Hernández, Q., Badías, A., Chinesta, F., and Cueto, E. Thermodynamics informed Graph Neural Networks. IEEE Transactions on Arti

cial Intelligence, DOI 10.1109/TAI.2022.3179681, 2022.

[3] Hernández, Q., Badías, A., Chinesta, F., and Cueto, E. Port-metriplectic neural networks: thermodynamics-informed machine learning of complex physical systems. arXiv preprint arXiv:2211.01873, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Polyconvex hyperelasticity and electro-elasticity with physics-augmented neural networks

Dominik K. Klein*, Rogelio Ortigosa§, Jesús Martínez-Frutos§, and Oliver Weeger*

*Cyber-Physical Simulation Group & Graduate School of Computational Engineering
Technical University of Darmstadt
Darmstadt, Germany
e-mail: klein@cps.tu-darmstadt.de

§Technical University of Cartagena
Cartagena (Murcia), Spain

Keywords: constitutive modeling, multiscale simulation, physics-augmented neural networks, polyconvexity, nonlinear electro-elasticity

In the last decades, a vast amount of highly specialized metamaterials has been developed and, with advancing requirements in engineering applications, the trend is growing. Comprised of complex microstructures, these materials can be tailored for each specific application. At the same time, this sets a challenge for the mechanical description of such materials, as they behave highly nonlinear. Thus, we envision the use of physics-enhanced neural networks, circumventing the current limitations of analytically formulated material models. In the present work [1], two machine learning based constitutive models for finite deformations are proposed. Using input convex neural networks, the models are hyperelastic, anisotropic and fulfill the polyconvexity condition, which implies ellipticity and thus ensures material stability.

The first constitutive model is based on a set of polyconvex, anisotropic and objective invariants. The second approach is formulated in terms of the deformation gradient, its cofactor and determinant, uses group symmetrization to fulfill the material symmetry condition, and data augmentation to fulfill objectivity approximately. The extension of the dataset for the data augmentation approach is based on mechanical considerations and does not require additional experimental or simulation data. The models are calibrated with highly challenging simulation data of cubic lattice metamaterials, including finite deformations and lattice instabilities. A moderate amount of calibration data is used, based on deformations which are commonly applied in experimental investigations. While the invariant-based model shows drawbacks for several deformation modes, the model based on the deformation gradient alone is able to reproduce and predict the effective material behavior very well and exhibits excellent generalization capabilities. In addition, the models are calibrated with transversely isotropic data, generated with an analytical polyconvex potential. For this case, both models show excellent results, demonstrating the straightforward applicability of the polyconvex neural network constitutive models to other symmetry groups.

Finally, the invariant-based model is extended towards electro-mechanically coupled material behavior at finite deformations [2], see Fig. 1. Now using electro-mechanically coupled invariants, the model fulfills the material stability condition, as well as thermodynamic consistency, objectivity, material symmetry, and growth conditions. Depending on the con-

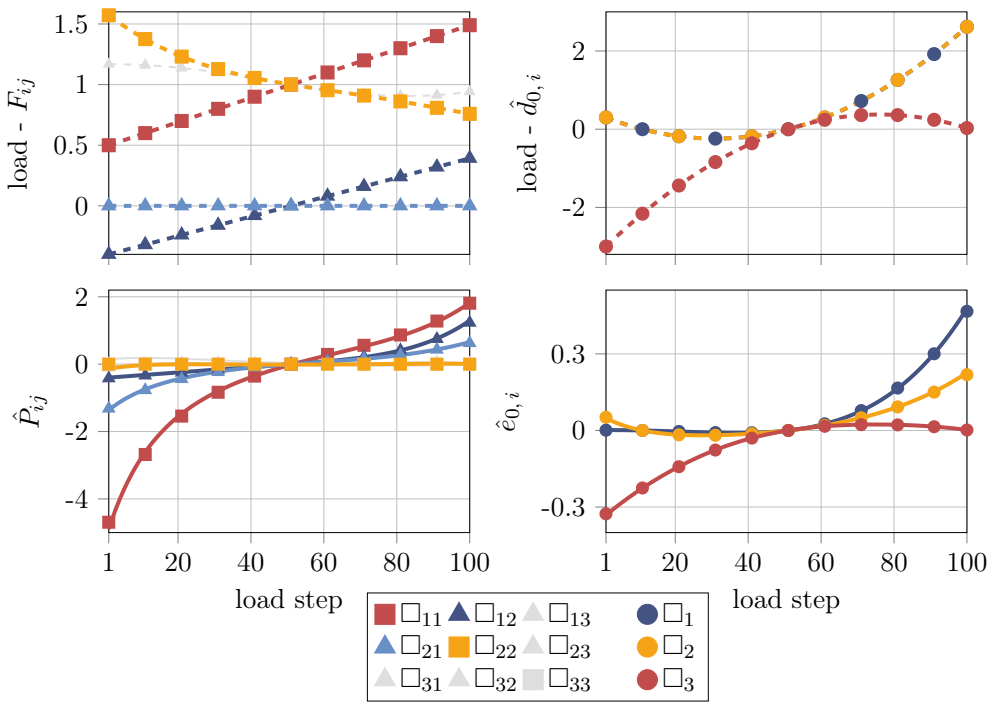


Figure 1: Model prediction for a homogenized, electro-mechanical rank-one laminate. Points depict homogenization data, while lines depict the evaluation of the machine learning model. The load (upper figures) consists of both complex mechanical and electrical load, and both the mechanical stress $\boldsymbol{P}$ and electric field $\boldsymbol{e}$ are predicted excellent (lower figures).

sidered invariants, this physics-enhanced machine learning model can either be applied for compressible or nearly incompressible material behavior, as well as for arbitrary material symmetry classes. This extension towards multiphysical material behavior shows once again the efficiency and robustness of our approach. Recently, the models are extended towards inelastic material behavior and applied for efficient multiscale simulation.

References

[1] D. K. Klein, M. Fernández, R. J. Martin, P. Neff, O. Weeger. Polyconvex anisotropic hyperelasticity with neural networks. JMPS 159:104703 (2022).

[2] D. K. Klein, R. Ortigosa, J. Martínez-Frutos, O. Weeger. Finite electro-elasticity with physics-augmented neural networks. CMAME 400:115501 (2022).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A recurrent machine learning structure for few-shot constitutive model optimization: Application to Geomechanics

Shaoheng Guan* **and Sascha Ranftl†**

* Institute of Theoretical Physics-Computational Physics
Graz University of Technology, Petersgasse 16, 8010 Graz, Austria
e-mail: shaohengguan@gmail.com, ranftl@tugraz.at

Abstract: In practice, a purely data-driven approach for building a generic 2D or 3D stress-strain relationship without introducing physical constraints (assumptions) is rather difficult to be embedded in boundary value problems' (BVP) calculations, as the strain paths may be highly variable. With machine learning (ML)-based constitutive models, it is not the 'best' predictions that lead to the success of the computation, but, conversely, rather the worst predictions that often lead to the failure of the computation. To address the problem of insufficient generalization, the material 'cell' is proposed with the assumptions of the so-called Critical-State-Unified-Hardening (CSUH) [1] model working as the physics constrains in the PyTorch framework. Based on strain-stress sequence data from explicit FEM-DEM (exFEM-DEM) simulations, the parameters of a material 'cell' were optimized with the Adam algorithm and error backpropagation. Eight sets of $(\epsilon_{ij} - \sigma_{ij})$ sequences in one exFEM-DEM BVP simulation are used for model training, and two different BVP simulations are utilised to assess the optimized model.

Keywords: Machine Learning, Constitutive Modeling, Granular Materials, FEM-DEM, Optimization

1 Introduction

With the advent of ML, especially neural networks ($\mathcal{NN}$), recent research focuses on rebuilding constitutive models (i.e. mapping $\epsilon_{ij} \rightarrow \sigma_{ij}$) via ML methods. However, it is impossible to cover the entire $(\epsilon_{ij}, \mathcal{I})$-space without simplifying assumptions. Such models are known to generalize poorly, and high prediction errors can cause BVP calculations to become nonsensical and/or crash. Most studies focus on improving the best prediction accuracy. But, unfortunately, there is rarely a proper method to guarantee the ML model's poorest performance is above some acceptable threshold. Here we introduce the CSUH model as the physical constraint for the ML model to improve the generalization.

2 Methodology

All constitutive models can generally be represented as

$$\mathcal{I} = \mathcal{M}\left(\dot{\epsilon}_{ij}, \mathcal{I}_0\right) \ , \tag{1}$$

where $\mathcal{I}$ is the set of state variables, including but not limited to the stress tensor σ_{ij}, $\mathcal{I}_0$ is the initial state before the strain increment $\dot{\epsilon}_{ij}$, and $\mathcal{M}$ is the material 'cell' employed in the recurrent structure, as is shown in Fig. 1(a). This equation is very similar to the recurrent neural network format $h = \mathrm{RNNCell}(x, h_0)$, where RNNCell is a network cell, x is the

input, h is the hidden state (Fig. 1(b)). This implies that the training process of $\mathcal{M}$ is very similar to the training process of a recurrent neural network given the CSUH-assumptions, i.e. $\mathcal{M} \triangleq$ RNNCell | CSUH formulas.

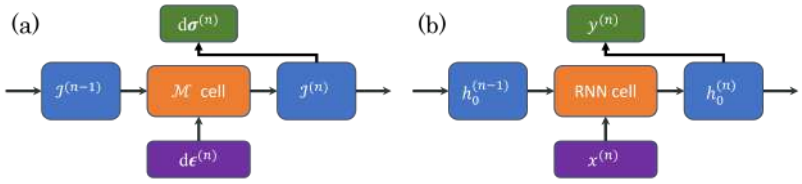


Figure 1: The comparison of the architecture of the material cell and a RNN cell-based ML method

3 Conclusions

The comparison of biaxial compression simulations is displayed in Fig. 2. The curves of maximum a mean the largest value among all of the accelerations of the nodes.

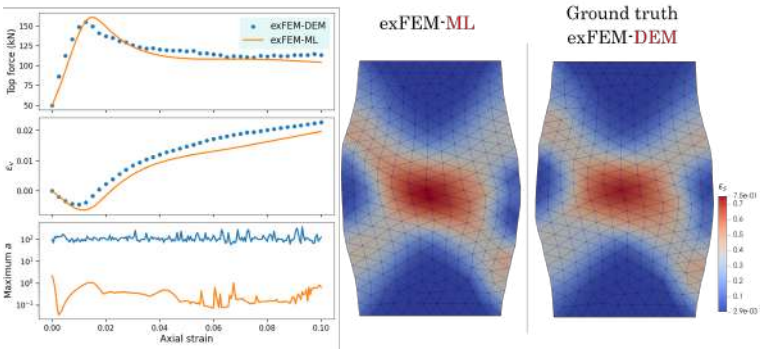


Figure 2: Comparison of the biaxial compression in exFEM-DEM and exFEM-ML

The physics-constrained $\mathcal{M}$-cell trained on the datasets collected from the exFEM-DEM simulations can be used to properly reproduce the exFEM-DEM simulation under various circumstances. The physics constraints are effectively implemented by recognizing the state equations with the training process of a recurrent structure and improving the model's generalization [2]. Recurrent neural networks are known to induce a corresponding Gaussian process [3], posing a possible route for incorporating further prior knowledge on the underlying PDE [4].

References

[1] Y.P. Yao et al. "Unified hardening (UH) model for clays and sands," Comput. Geotech. (2019), vol. 110, no. March, pp. 326–343,

[2] S. Guan et al. "A machine learning-based multi-scale computational framework for granular materials", Acta Geotechnica (2022)

[3] S. Xian et al. "Recurrent neural network-induced Gaussian process", Neural Computing (2022), vol. 509, pp. 75-84

[4] S. Ranftl "A connection between probability, physics and neural networks". Phys. Sci. Forum (2022), vol. 5, no. 11

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Prediction of Flow Fields in Bioreactors with Physics-Informed Neural Networks

Veronika Travnikova*, Nico Dirkes*, Eric von Lieres† and Marek Behr*

*Chair for Computational Analysis of Technical Systems (CATS)
RWTH Aachen University
Aachen, Germany
e-mail: travnikova@cats.rwth-aachen.de

† Institute of Bio- and Geosciences (IBG-1)
Forschungszentrum Jülich
Jülich, Germany

Abstract: This work aims to investigate the applicability of Physics-Informed Neural Networks to construct Reduced Order Models for predicting flow fields in bioreactors. To improve accuracy of the predictions, approaches such as domain decomposition based on the distinct character of the flow in different parts of the domain and hard imposition of boundary constraints are leveraged. Models capable of prediction within a range of Reynolds numbers were trained.

Keywords: Physics-Informed Neural Networks, CFD, Navier-Stokes Equations, Reduced Order Models

1 Introduction

Fermentation in bioreactors is an essential tool in biotechnological research and production. Since there is little information available on the production processes and environmental conditions of the cells due to the lack of suitable measurement techniques, Computational Fluid Dynamics (CFD) is often used to simulate flow fields in bioreactors and enable the prediction of velocity and pressure, as well as specific characteristics, such as mixing times. The computational intensity of high-fidelity simulations in scenarios, where the same model must be solved multiple times for different parameter values motivates the construction of Reduced Order Models (ROMs) to approximate solutions at a lower computational cost. Physics-Informed Neural Networks (PINNs), originally proposed by Raissi et al. [1], are a promising candidate for ROMs in engineering problems, where data is typically sparse and costly to obtain, and the governing equations are known.

2 Methods

Physics-informed neural networks aim to reduce the amount of data needed to learn the solution of a problem by embedding its governing equations (in this case Navier-Stokes equations) and boundary constraints into the loss function. The cross-section of a bioreactor in the impeller plane is considered as the computational domain for a two-dimensional model. The stirring of the bioreactor is simulated by prescribing a linear velocity profile on the impeller blades from the center outwards and the model captures a snapshot of one specific time instance, at which the impeller blades are exactly aligned with the cartesian coordinate

axis. The predictive accuracy of the model can be improved, e.g., by imposing boundary constraints in a post-processing step using an interpolation spline or by leveraging additional knowledge of the problem and decomposing the computational domain based on the distinct character of the flow in different parts of the domain [2].

3 Results

Figure 1 shows the results of a two-dimensional bioreactor model parameterized by the stirring rate, described by the dimensionless Reynolds number *Re*. The prediction accuracy of the model was evaluated by comparison to high-fidelity CFD simulation results. The model achieves a mean relative velocity error of 1–3% w.r.t. the impeller tip velocity depending on the value of *Re*.

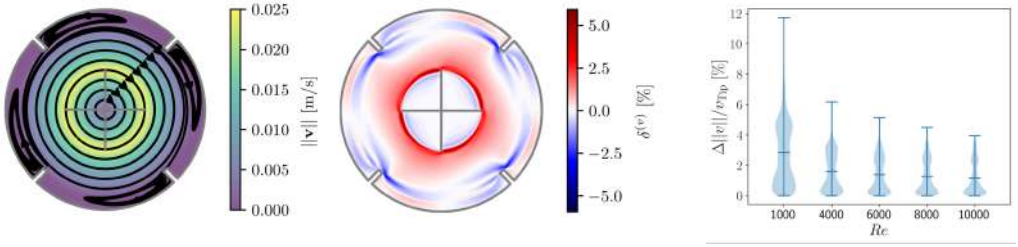


Figure 1: Velocity field (left), relative velocity error distribution in the computational domain (center) and relative velocity error for *Re* in the range $10^3 - 10^4$ (right) in a bioreactor predicted by a PINN.

4 Conclusions

The applicability of PINNs as reduced simulation models for bioreactors was investigated. The prediction accuracy of a 2D bioreactor model parameterized by *Re* was improved significantly by employing approaches such as domain decomposition and hard imposition of boundary constraints. The strategies tested in the presented use case will be applied to 3D models.

5 Acknowledgements

This work was performed as part of the Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE) and received funding from the Helmholtz Association of German Research Centres.

References

[1] Raissi M, Perdikaris P, Karniadakis GE. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. J Comput Phys 2019;378:686-707.

[2] Dirkes N. Advanced Strategies for Improving Physics-Informed Neural Networks as Reduced Simulation Models. Master thesis. RWTH Aachen University 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A Surrogate Model for Prediction of Vibrations Induced by Impact Pile Driving

M. Abouelmaty. A[*†], Colaço. A[†], Alves Costa. P[†]

[†] Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
Corresponding e-mail: up201903008@fe.up.pt

[*] Department of Construction and Building Engineering (CB)
College of Engineering and Technology, Arab Academy for Science, Technology & Maritime Transport
Alexandria, Egypt

Abstract: Pile driving activities in urban areas can generate excessive ground-borne vibrations and interfere with people and structures in the vicinity. During the foundation's design stage, it is desirable to have expedite methodologies for the prediction of vibrations in a simple and quick-to-compute. This work presents the proceeding followed for developing a surrogate model based on Artificial Neural Networks, ANNs, able to predict ground-borne vibrations induced by pile-driving.

Keywords: Artificial Neural Network; surrogate model; Ground-borne vibrations; Pile Driving.

1. INTRODUCTION

In various construction sites, vibrations are considered a critical aspect. In particular, vibrations generated from the installation of driven piles can reach higher levels when compared with current standard limits. Predicting ground vibrations due to pile driving is a complex problem that is affected by many factors, e.g., energy transmitted from the hammer to the pile, geotechnical conditions of the site, distance from the source, soil-structure interaction, among others. Different methodologies can be employed in this task, from empirical approaches to detailed and complex numerical formulations. This work intends to present a prediction methodology based on machine learning techniques that emulate the complex model, looking for a versatile and accurate tool.

From this context, the author aims to introduce an ANN model for predicting peak particle velocities (PPV) values at the ground surface induced by the pile driving process. ANNs introduce adequate abilities to deal with the complex behaviors of the pile-ground system. The data quality inside the learning database, which will be used in training the ANNs model, controls the accuracy level of the ANNs model. Therefore, an axisymmetric FEM-PML numerical model would be used for the purpose of generating the learning database [1].

2. METHODOLOGY AND RESULTS

An axisymmetric FEM-PML numerical model was used to generate the database, which contains a total of 1400 cases. These cases are addressed within the input parameters in an identified ranges. The input parameters are correlated to pile properties, soil properties, and hammer properties. After modeling the learning database, it is essential to remove the influence of the numbers using standardization and linearization techniques. The essentiality of this step arises from the fact that the contrast between the mean values of the input parameters can conduct to misleading the algorithm throughout escalations of some parameters rather than others.

The next step in building the ANNs model is dividing the learning database into subsets. Every subset has its utilizing, characterizing, and influence on the final output results. These

subsets are the training, testing, and validation sets. The training set is used to train a model, the validation set is used to evaluate the model during training, and the test set is used to evaluate the model after it has been trained.

The training of the ANNs model would be performed on the Matlab® program. The properties of the trained model were placed under a set of training iterations in order to find the most proper combination that shows the lowest R^2 value. The ANN architecture consisted of an input layer, one hidden layer with three nodes, and an output layer. The dividing ratio of the learning database is 70%, 10%, and 20% for training, testing and validation sets, respectively. The fitting training algorithm in Matlab used was "Levenberg-Marquardt".

A case study is exposed for the purpose of presenting the matching between the numerical model and ANNs model (see Figure 1). The input parameters of the case study were within the learning database's boundary limits and were modeled using FEM-PML numerical model and ANNs model. The figure verified an adequate matching between the FEM-PML numerical model and the ANNs model. Such matching gives the generated ANNs model reliability in instantaneous prediction for the vibration induced by the pile driving process with an acceptable accuracy level.

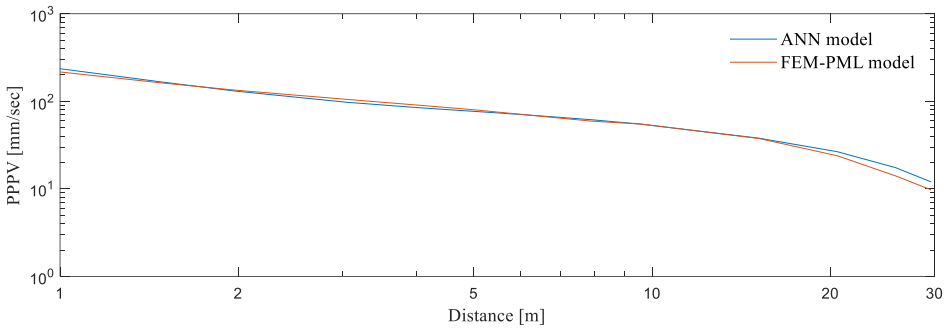


Figure 1: The axisymmetric FEM-PML numerical model vs. ANNs model prediction comparison.

3. FINAL CONCLUSIONS

From the results achieved, it is evident a remarkable agreement between ANNs model and numerical results. Even though the ANNs model was carried out under limited scope, the model is able to address the main features of the problem. In further works, the ANNs model presented will be upgraded for the prediction of the frequency content of the response.

Acknowledgements

This work was financially supported by: Base Funding - UIDB/04708/2020 and Programmatic Funding - UIDP/04708/2020 of the CONSTRUCT - Instituto de I&D em Estruturas e Construções – funded by national funds through the FCT/MCTES (PIDDAC); National funds through the FCT/MCTES (PIDDAC), under the project PTDC/ECI-EGC/3352/2021; Individual Grant No. 2022.11639.BD.

References

[1] Colaço, A, P Alves Costa, C Mont'Alverne Parente, and A Silva Cardoso. 2021. "Ground-Borne Noise and Vibrations in Buildings Induced by Pile Driving: An Integrated Approach." Applied Acoustics 179: 108059.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A hybrid AI based approach for the optimization of composite coatings development through electroplating processes

Andrea Gregores Coto, Christian Eike Precker and Santiago Muiños-Landin*

* Smart Systems and Smart Manufacturing (S3M) Group,
Artificial Intelligence and Data Analytics Laboratory (AIDALab), AIMEN Technology Centre
36440 O Porriño, Spain
e-mail: santiago.muinos@aimen.es

Abstract: This work presents a methodology relying on Artificial Intelligence (AI) and modelling methods to improve the synthesis of new coating solutions for the surface finishing industry. Such methodology is based on the development of a hybrid dataset composed of experimental data of electroplating processes and also computational models. These models describe the hydrodynamics of the system on the one hand, and the coating deposition on the other. Such dataset is used with two main purposes: first, feeding a Generative Model (GAN) for the design and optimization of the electrolytic bath and second, to feed a Physics Informed System (PINN) that predicts properties of the coating deposition for a set of electrochemical conditions. The present work describes the structure of the dataset and the main approaches followed to construct the GAN and the PINN networks for each case. This methodology represents a remarkable step towards the definition of a safe and sustainable by design (SSbD) framework for the development of composite coatings that can replace hard chromium, known as a toxic component, for applications in manufacturing, machinery and the automotive industry.

Keywords: Artificial Intelligence, Generative Models, Physcis Informed Systems, Material Science

1. Introduction

In order to enhance materials performance in different applications, metal coatings are typically deployed to improve features such as corrosion resistance, colour, wear resistance, electrical resistance, optical properties, or thermal behavior. However, nowadays hard chromium, known as a toxic and cancinogenic substance, is widely used on such metallic coatings that are demanded in sectors from building and construction to automotomotive and consumer goods. This represents an inconvenience for the deployment of metallic coatings as a part of a sustainable manufacturing chain. Which means that these improvements that in metallic coatings could be achieved by means of a materials design framework that addresses the safety and the sustainability of the product from the beginning and considering the entire material lifecycle. Such framework can be only achieved with the help of in silico approaches relying on computational methods and Artificial Intelligence that triggers the generation and exploitation of large amount of data that typically involves remarkable resources if only experimental methods are involved.

This work presents some parts of such in silico approaches as a piece of a safe and sustainable by design (SSbD) framework for the development of composite coatings within the framework of the EU funded MOZART project (GA **101058450).** Which has the purpose of assisting the fulfillment of industrial requirements of metallic coatings while eliminating Hard Chromium (HC) and offering a Nickel matrix nanocomposite[1] electroplating process. Which represents an environmentally less harm and less toxic alternative to the painting and coating industry, following the SSbD principles.

2. Content

While the global in silico approach followed by the entire methodology is composed by computational models and AI methods, this work addresses only the description of the AI techniques developed in order to address the design of the electrolytic bath for the optimal electroplating process and also the prediction of coating properties. The work involves the design of the bath including the presence of nanoparticles and also 2D nanomaterials. The first part is addressed by the definition of Generative models (Generative Adversarial Networks (GAN) see Fig. 1)[2] while for the second, a Physics Informed Neural Network (PINN)[3] has been defined. In this work we also address the design of the dataset needed to train these networks. Within the context of the Mozart project, a hybrid dataset has been created based on experimental data but also synthetic data coming from the computational models developed within the project.

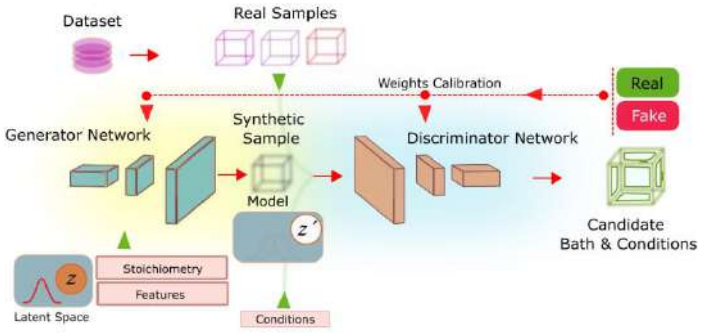


Figure 1. General architecture of the GAN developed to drive the design of the electrolytic bath and it physical condition.

4. Outcome

The hybrid dataset is presented and described in this work. Such dataset leads to the definition of the architecture of the two networks needed to design the electrolytic bath and its physical conditions (GAN) and to predict the coating properties for a given electroplating conditions. (PINN). The network architectures are presented and performances are evaluated.

Acknowledgements

This research has received funding from the European Union's Horizon Europe research and innovation programme under the project Mozart with Grant Agreement 101058450. The authors want to thank the comments and fruitful discussions with all the members of the Artificial Intelligence and Data Analytics Lab (AIDA-Lab) of the Smart Systems and Smart Manufacturing (S3M) department of the AIMEN Technology Centre.

References

[1] M. Malaki, "Advanced Metal Matrix Nanocomposites", Metals, (9) p.330, 2019

[2] Y. Dan *et al.* Generative adversarial networks (GAN) based efficient sampling of chemical composition space for inverse design of inorganic materials. *npj Comput Mater* **6**, 84, 2020

[3] M. Raissi, P. Perdikaris, G.E. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics, Volume 378, 2019

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Improving Physics Informed Neural Network: alternative approaches to enforce Dirichlet boundary conditions

Pintore Moreno*, Berrone Stefano*, Canuto Claudio* and Sukumar Natarajan†

* Dipartimento di Scienze Matematiche (DISMA)
Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy
e-mail: stefano.berrone@polito.it, claudio.canuto@polito.it, moreno.pintore@polito.it

† Department of Civil and Environmental Engineering
University of California, Davis, CA 95616, USA
e-mail: nsukumar@ucdavis.edu

Abstract: In this work, we propose and compare strategies to enforce Dirichlet boundary conditions in Physics Informed Neural Networks and Variational Physics Informed Neural Networks. In these models, Dirichlet boundary conditions are usually enforced by means of additional terms in the loss function to penalize the difference between the model output and the prescribed condition. We propose alternative strategies based on approximate distance functions to exactly enforce the BCs, without the need to learn them, and a variational approach to weakly impose them (via Nitsche's method), that does not lead to a multiobjective loss function. Such strategies are not problem dependent and can be applied to any partial differential equation on convex or non-convex domains. Numerical results on various differential problems are presented. We show that exactly enforcing the BCs via approximate distance functions is the best approach since it leads to more accurate and efficient solvers and does not rely on any tunable hyper-parameter.

Keywords: Dirichlet boundary conditions, PINN, VPINN, Approximate distance function, Nitsche's method

1 Introduction

After the first paper of Raissi et al. [1], Physics Informed Neural Networks (PINNs) are rapidly emerging as a flexible deep learning method to solve partial differential equations (PDEs). In order to improve the original PINN formulation, several extensions have been developed. In this work we only focus on the original PINN and on the interpolated Variational Physics Informed Neural Network (VPINN) proposed in [2] (that is an extension of the standard VPINN [3]), which relies on the weak formulation of the PDE.

In order to compute an approximate solution, a neural network is trained to minimize the residual of the PDE on a given set of collocation points and, in general, a penalization term is added to the loss function in order to enforce the required BCs. In this work, instead, we propose and compare three alternative approaches to enforce Dirichlet BCs. Two of them are used to exactly enforce them via approximate distance functions [4], whereas the third one weakly enforce them via Nitsche's method [5].

2 Extended abstract content

In this work, we compare the performance of PINNs and interpolated VPINNs on different problems and enforcing the Dirichlet BCs in different ways. The main difference between

these two models is that the PINN loss function is computed using the residual of the strong formulation of the PDE, whereas the VPINN one is obtained from the weak formulation. In such a formulation, the involved test functions are piecewise linear functions defined on a suitable triangulation.

We present two strategies to exactly enforce Dirichlet BCs on both PINNs and VPINNs adding a non-trainable layer at the end of the neural network. Such strategies can be extended as in [4] to enforce other types of BCs. Then, we also show how to weakly enforce Dirichlet BCs in VPINNs exploiting the variational nature of the residuals. We highlight that such approaches do not require any possibly expensive tuning phase, that may be needed if the BCs are enforced via an additional cost in the loss function.

3 Conclusions

The strategies are tested on various PDEs. We observe that exactly enforcing the Dirichlet BCs using approximate distance functions is convenient to reduce training time and increase the model accuracy. Instead, if other functions are adopted, one observes suboptimal performance. Poor performances are also observed when Nitsche's method is used.

The presented strategies and numerical experiments are discussed in greater detail in [6].

References

[1] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics, 378:686–707, 2019

[2] S. Berrone, C. Canuto, M. Pintore, Variational physics informed neural networks: the role of quadratures and test functions, Journal of Scientific Computing 92 (2022) 1–27.

[3] E. Kharazmi, Z. Zhang, G. Karniadakis, hp-VPINNs: Variational physics-informed neural networks with domain decomposition, Computer Methods in Applied Mechanics and Engineering 374 (2021) 113547.

[4] N. Sukumar, A. Srivastava, Exact imposition of boundary conditions with distance functions in physics-informed deep neural networks, Computer Methods in Applied Mechanics and Engineering 389 (2022) 114333.

[5] J. A. Nitsche, Uber ein Variationsprinzip zur Losung Dirichlet-Problemen bei Verwendung von Teilraumen, die keinen Randbedingungen unteworfen sind, Abh. Math. Sem. Univ., Hamburg 36 (1971) 9–15.

[6] S. Berrone, C. Canuto, M. Pintore, N. Sukumar, Enforcing Dirichlet boundary conditions in physics-informed neural networks and variational physics-informed neural networks, arXiv preprint arXiv:2210.14795 (Unpublished results - Submitted).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Mathematical and computational modeling of the electro-mechano-fluid activity of the heart

Michele Bucelli[*,1], **Alberto Zingaro**[1], **Pasquale Claudio Africa**[1], **Ivan Fumagalli**[1], **Luca Dede'**[1], **Alfio Quarteroni**[1,2]

[*] Corresponding author. E-mail: michele.bucelli@polimi.it

[1] MOX, Dipartimento di Matematica, Politecnico di Milano, P.zza Leonardo da Vinci 32, 20133 Milan, Italy

[2] Institute of Mathematics, École Polytechnique Fédérale de Lausanne, Station 8, Av. Piccard, CH-1015 Lausanne, Switzerland (Professor Emeritus)

Abstract: We present a mathematical model that couples cardiac electrophysiology, active and passive mechanics, blood hemodynamics and the circulatory system, with the aim of reproducing the behavior of a human heart. We combine existing state-of-the-art models for the individual components of the heart function into an integrated mathematical and computational framework, introducing suitable numerical methods to deal with the coupling. The computational framework is applied to the simulation of a realistic human heart, comparing the results obtained with data from the medical literature, in qualitative and quantitative terms. The results indicate that the model has the potential of reproducing the physiological behavior of the heart.

Keywords: heart modeling, multiphysics, fluid-structure interaction, hemodynamics

1 Introduction

Computational modeling is an increasingly used tool for the study the heart function in physiological and pathological conditions [1, 2]. We propose a fully coupled model that describes cardiac electrophysiology, active and passive muscular mechanics and three-dimensional blood hemodynamics, leveraging state-of-the-art models and methods and combining them in an integrated computational framework. The model is validated by comparing numerical results against data from the medical literature.

2 Models and methods

We model cardiac electrophysiology with the monodomain equation. Active muscular mechanics is modeled with the biophysically detailed RDQ20-MF force generation model [3], and passive mechanics is described combining the Guccione and neo Hooke constitutive laws. Blood hemodynamics is represented by the Navier-Stokes equations in ALE formulation, using the RIIS method to account for the presence of valves [4]. We include electro-mechanical and mechano-electrical feedback, the feedback between contraction and fiber shortening, as well as fluid-structure interaction. We bi-directionally couple the blood flow with a lumped model for the circulatory system. We solve the resulting multiphysics problem with finite elements in a segregated-staggered approach, treating the fluid-solid coupling in a monolithic way [5].

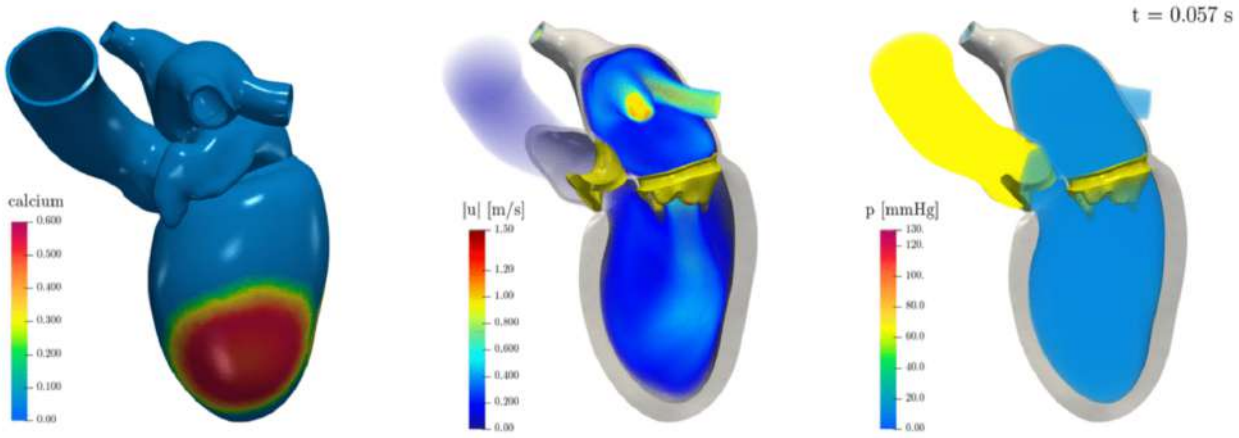


Figure 1: From left to right: intracellular calcium concentration, blood velocity and blood pressure in a left heart simulation.

3 Numerical results

We simulate a realistic left heart and a whole heart model, obtaining results that are in qualitative agreement with the behavior observed in medical images. Quantitative indicators such as chamber volumes, pressures and flow rates through the cardiac valves also match physiological data from the medical literature.

Acknowledgements: This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 740132, iHEART - An Integrated Heart Model for the simulation of the cardiac function, P.I. Prof. A. Quarteroni).

References

[1] Michele Bucelli, Alberto Zingaro, et al. A mathematical model that integrates cardiac electrophysiology, mechanics and fluid dynamics: application to a human left heart. *Int J Num Meth Biomed Eng*, 2022.

[2] Alfio Quarteroni, Luca Dede', Andrea Manzoni, and Christian Vergara. *Mathematical modelling of the human cardiovascular system: data, numerical approximation, clinical applications*, volume 33. Cambridge University Press, 2019.

[3] Francesco Regazzoni, Luca Dede', and Alfio Quarteroni. Biophysically detailed mathematical models of multiscale cardiac active mechanics. *PLoS Comp Biol*, 16(10):e1008294, 2020.

[4] Marco Fedele, Elena Faggiano, et al. A patient-specific aortic valve model based on moving resistive immersed implicit surfaces. *Biomech Model Mechanobiol*, 16(5):1779–1803, 2017.

[5] Michele Bucelli, Luca Dede', et al. Partitioned and monolithic FSI schemes for the numerical simulation of the heart. *Comm Comput Phys (in press)*, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Finite element discretization of fluid-structure interaction problems with fictitious domain approach

Daniele Boffi[*,†], **Fabio Credali**[†,*] **and Lucia Gastaldi**[‡]

[*] Computer, Electrical and Mathematical Sciences and Engineering Division (CEMSE)
King Abdullah University of Science and Technology
23955, Thuwal, Saudi Arabia
e-mail: daniele.boffi@kaust.edu.sa

[†] Dipartimento di Matematica "F. Casorati"
Università degli Studi di Pavia
27100, Pavia, Italy
e-mail: fabio.credali01@universitadipavia.it

[‡] Dipartimento di Ingegneria Civile, Architettura, Territorio, Ambiente e di Matematica (DICATAM)
Università degli Studi di Brescia
25123, Brescia, Italy
e-mail: lucia.gastaldi@unibs.it

Abstract: We present advances on a fictitious domain formulation for fluid-structure interaction problems based on Lagrange multiplier. The finite element discretization of the coupling matrix is defined through integration of functions defined over non-overlapping meshes: after introducing two techniques one can adopt to carry out this procedure, we present error estimates for the quadrature error.

Keywords: fluid-structure interactions, fictitious domain, finite elements, non-overlapping meshes

1 Introduction

We discuss a computational aspect regarding a fictitious domain formulation for fluid-structure interaction problems born as evolution of the immersed boundary method [1]. We denote by Ω_t^f and Ω_t^s the two regions in $\mathbb{R}^{d=2,3}$ occupied, at the time instant t, by the fluid and the solid respectively. In particular, the fluid is extended into $\Omega = \Omega_t^f \cup \Omega_t^s$ in order to occupy also the region occupied by the solid. In Ω, the dynamics of a Newtonian fluid, with velocity $\mathbf{u}$ and pressure p, is governed by the incompressible Navier–Stokes equations on a fixed mesh with Eulerian description. On the other hand, for the immersed hyper-elastic solid, we adopt the Lagrangian description by introducing a reference domain $\mathcal{B}$, which is mapped into the actual position of the solid body via a function $\mathbf{X} : \mathcal{B} \longrightarrow \Omega_t^s$ such that each $\mathbf{x} \in \Omega_t^s$ can be described by $\mathbf{x} = \mathbf{X}(\mathbf{s}, t)$, with $\mathbf{s} \in \mathcal{B}$. In particular, in this fictitious domain setting, we impose that the material velocity is equal to $\mathbf{u}$ in Ω_t^s, therefore $\mathbf{u}(\mathbf{X}(\mathbf{s}, t), t) = \partial \mathbf{X}(\mathbf{s}, t)/\partial t$ for $\mathbf{s} \in \mathcal{B}$. This constraint is weakly imposed making use of a Lagrange multiplier: for this purpose, we introduce a functional space $\mathbf{\Lambda}$ on $\mathcal{B}$ and a continuous bilinear form $\mathbf{c} : \mathbf{\Lambda} \times (H^1(\mathcal{B}))^d \longrightarrow \mathbb{R}$ characterized by the fact that if $\mathbf{c}(\boldsymbol{\mu}, \mathbf{Y}) = 0$ for all $\boldsymbol{\mu} \in \mathbf{\Lambda}$, then $\mathbf{Y} = 0$.

Since, as described in [2], the time semi-discretized version of an FSI problem can be seen a sequence of stationary problems, we reduce our analysis to this case. Therefore, we define

two bilinear forms, one for the fluid and one for the solid,

$$\mathbf{a}_f(\mathbf{u},\mathbf{v}) = \alpha(\mathbf{u},\mathbf{v})_\Omega + \nu(\boldsymbol{\nabla}_{\mathrm{sym}}(\mathbf{u}),\boldsymbol{\nabla}_{\mathrm{sym}}(\mathbf{v}))_\Omega + \frac{\rho_f}{2}\oint(\overline{\mathbf{u}}\cdot\boldsymbol{\nabla}\,\mathbf{u},\mathbf{v})_\Omega - (\overline{\mathbf{u}}\cdot\boldsymbol{\nabla}\,\mathbf{v},\mathbf{u})_\Omega\big) \quad \forall \mathbf{u},\mathbf{v}\in(H^1_0(\Omega))^d$$

$$\mathbf{a}_s(\mathbf{X},\mathbf{Y}) = \beta(\mathbf{X},\mathbf{Y})_\mathcal{B} + \gamma(\boldsymbol{\nabla}_{\mathrm{s}}\,\mathbf{X},\boldsymbol{\nabla}_{\mathrm{s}}\,\mathbf{Y})_\mathcal{B} \quad \forall \mathbf{X},\mathbf{Y}\in(H^1(\mathcal{B}))^d$$

so that, we can introduce the following problem.

Problem 1 *Let* $\overline{\mathbf{X}}\in(W^{1,\infty}(\mathcal{B}))^d$ *be invertible with Lipschitz inverse and* $\overline{\mathbf{u}}\in(H^1_0(\Omega))^d$ *such that* $\operatorname{div}\overline{\mathbf{u}}=0$. *Given* $\mathbf{f}\in(L^2(\Omega))^d$, $\mathbf{g}\in(L^2(\mathcal{B}))^d$ *and* $\mathbf{d}\in(H^1(\mathcal{B}))^d$, *find* $(\mathbf{u},p)\in(H^1_0(\Omega))^d\times L^2_0(\Omega)$, $\mathbf{X}\in(H^1(\mathcal{B}))^d$ *and* $\boldsymbol{\lambda}\in\boldsymbol{\Lambda}$, *such that*

$$\mathbf{a}_f(\mathbf{u},\mathbf{v}) - (\operatorname{div}\mathbf{v},p)_\Omega + \mathbf{c}(\boldsymbol{\lambda},\mathbf{v}(\overline{\mathbf{X}})) = (\mathbf{f},\mathbf{v})_\Omega \qquad \forall\mathbf{v}\in(H^1_0(\Omega))^d \tag{1a}$$

$$(\operatorname{div}\mathbf{u},q)_\Omega = 0 \qquad \forall q\in L^2_0(\Omega) \tag{1b}$$

$$\mathbf{a}_s(\mathbf{X},\mathbf{Y}) - \mathbf{c}(\boldsymbol{\lambda},\mathbf{Y}) = (\mathbf{g},\mathbf{Y})_\mathcal{B} \qquad \forall\mathbf{Y}\in(H^1(\mathcal{B}))^d \tag{1c}$$

$$\mathbf{c}(\boldsymbol{\mu},\mathbf{u}(\overline{\mathbf{X}})-\mathbf{X}) = \mathbf{c}(\boldsymbol{\mu},\mathbf{d}) \qquad \forall\boldsymbol{\mu}\in\boldsymbol{\Lambda} \tag{1d}$$

In particular, ρ_f denotes the density of the fluid, while ν represents the fictitious viscosity. Moreover, the constants α, β and γ derive from physical parameters and time step. We are assuming that the constitutive law of the solid material is linear.

2 The coupling term

The coupling between fluid and structure is represented by the term $\mathbf{c}(\boldsymbol{\mu},\mathbf{v}(\overline{\mathbf{X}}))$. Two possible choices for $\mathbf{c}$ are either the scalar product in $(L^2(\mathcal{B}))^d$ or in $(H^1(\mathcal{B}))^d$. Therefore, to build the finite element matrix, we need to integrate on $\mathcal{B}$ the product of $\boldsymbol{\mu}$, defined on a mesh for $\mathcal{B}$, with a velocity function $\mathbf{v}$, defined on a mesh for Ω and composed with $\overline{\mathbf{X}}$. In this way, the actual position of the body can be taken into account. Since the two involved meshes are non-matching in general, these computations are not trivial. In [3], we presented two possible techniques. First, one can compute exactly the coupling term by implementing a composite quadrature rule on a submesh of $\mathcal{B}$ obtained by computing the intersection between the fluid mesh and the solid one, mapped through $\overline{\mathbf{X}}$. Otherwise, one can directly integrate on each solid element, introducing an additional source of error. For the second case, estimates show that if the coupling is performed by the $(L^2(\mathcal{B}))^d$ scalar product, then the quadrature error linearly converges to zero. On the other hand, if $\mathbf{c}$ is the $(H^1(\mathcal{B}))^d$ scalar product, then there is no convergence, as already numerically shown in [3].

References

[1] Boffi, D., Cavallini, N., Gastaldi, L. The finite element immersed boundary method with distributed Lagrange multiplier. SIAM Journal on Numerical Analysis 53.6 (2015): 2584-2604.

[2] Boffi, D., Gastaldi, L. A fictitious domain approach with Lagrange multiplier for fluid-structure interactions. Numerische Mathematik 135.3 (2017): 711-732.

[3] Boffi, D., Credali, F., Gastaldi, L. On the interface matrix for fluid–structure interaction problems with fictitious domain approach. Computer Methods in Applied Mechanics and Engineering, Volume 401, Part B (2022): 115650.

FLUID-STRUCTURE INTERACTION OF SLENDER BODIES IMMERSED IN THREE-DIMENSIONAL FLOWS: A NEW APPROACH FOR MATHEMATICAL MODELLING AND NUMERICAL APPROXIMATION

Muriel Boulakia[1], Céline Grandmont[2,3], Miguel-Angel Férnandez[2], Fabien Lespagnol[4], Paolo Zunino[4]

[1] Université Paris-Saclay, UVSQ, Paris, France
[2] Laboratoire Jacques-Louis Lions, UMR 7597, Sorbonne Université & Centre de Recherche Inria de Paris, Paris, France
[3] Département de Mathématique, ULB, Bruxelles, Belgique
[4] MOX, Department of Mathematics, Politecnico di Milano, Milan, Italy

Key Words: *fluid-structure interaction, beam theory, mixed dimensional PDEs*

We leverage on a new framework to formulate and approximate coupled partial differential equations (PDEs) on manifolds with heterogeneous dimensionality [1,2,3]. We use our theoretical knowledge to investigate the mathematical formulation and develop numerical methods for fluid-structure interaction (FSI) that integrate 1D representation of slender structures with a 3D flow. The solutions of such problems are affected by low regularity, which in turn reduces the ability to construct convergent and efficient approximation methods. The new approach that we propose overcomes the previous issue because it has the fundamental advantage to enable the approximation of the problem using Galerkin projections on Hilbert spaces [1,2]. For this reason, we can perform a rigorous convergence analysis of approximation methods, such as the Finite Element Method (FEM), applied to these problems [1,2]. First, we address some general aspects of 3D-1D mixed dimensional PDEs, with particular attention to their coupling, achieved by means of Lagrange multipliers combined with a suitable projection operator form the 3D solution space to the 1D space. We analyse the reduced coupling strategy by studying simplified models and their asymptotic behavior [3]. Second, we apply this approach to the case of the interaction between single or multiple beams and an incompressible fluid, described as a 3D-1D FSI problem. For this example, we use a fictitious domain method in which the variational formulation of the flow problem is extended to the entire domain, thus overlapping the structure. Additionally, we perform the simulation on a non-conforming mesh, which allows us to write fluid and solid equations on domains independent of time. In this case, we propose and compare several explicit coupling schemes. We prove their stability in the energy norm, regardless of the ratio of fluid-structure density.

REFERENCES

[1] Laurino, F., Zunino, P. Derivation and analysis of coupled PDEs on manifolds with high dimensionality gap arising from topological model reduction (2019) *ESAIM: M2AN*, 53 (6), pp. 2047-2080.
[2] Kuchta, M., Laurino, F., Mardal, K.-A., Zunino, P. Analysis and approximation of mixed-dimensional PDEs on 3D-1D domains coupled with Lagrange multipliers (2021) *SINUM*, 59 (1), pp. 558-582.
[3] Boulakia, M., Grandmont, C., Lespagnol, F., Zunino, P., Reduced models for the Poisson problem in perforated domains, submitted, 2021.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Multiphysics and multiscale modeling of hemodynamics in arteries with in-stent restenosis

Anna Ranno*, Kiran Manjunatha †, Felix Vogt‡, Stefanie Reese† and Marek Behr*

* Chair for Computational Analysis of Technical Systems (CATS)
RWTH Aachen University, Germany
e-mail: {ranno, behr}@cats.rwth-aachen.de

†. Institute of Applied Mechanics (IFAM)
RWTH Aachen University, Germany
e-mail: {manjunatha, stefanie.reese}@ifam.rwth-aachen.de

‡ Department of Cardiology, Pulmonology, Intensive Care and Vascular Medicine
University Hospital RWTH Aachen, Germany
e-mail: fvogt@ukaachen.de

Abstract: The treatment of coronary artery disease most often involves coronary stents. Vessel injury after stent implantation can lead to in-stent restenosis and subsequent obstruction to the blood flow. In this work, we couple a multiphysics model for in-stent restenosis to hemodynamics and drug elution in stented arteries. To overcome different time scales between drug release, growth model, and blood flow, we adopt averaging techniques and adaptive time-stepping. We test our approach on a simplified ring stent geometry where we couple drug concentration, wall shear stress (WSS) and artery wall displacement at the fluid-solid interface.

Keywords: Stented Artery, In-Stent Restenosis, Coupled Problem, Drug Elution, Blood Flow

1 Introduction

The treatment of cardiovascular diseases most often involves coronary stents. Even with drug-eluting stents, implantation can often give rise to in-stent restenosis: endothelial denudation and overstretch injuries caused during the procedure kick-start various signaling cascades within the arterial wall resulting in uncontrolled tissue growth and formation of obstruction to the blood flow. Critical areas where such side effects occur highly depend on the shear stresses and drug distribution inside the artery. For this reason, the analysis of blood flow dynamics in stented arteries is of great interest. The current work is aimed at coupling hemodynamics and tissue growth to include the fluid-structure interaction of pharmacokinetics at the interface between artery and lumen.

2 Models

Navier Stokes equations and Newtonian constitutive model are used to simulate blood flow in a stented artery. Wall shear stress (WSS) related quantities are analyzed as indicators of the possible areas of inflammation and thrombosis. Particular emphasis is given to the influence of stent struts on microdynamics: recirculation areas and vortices are often located near the stent struts and their geometry strongly influences those flow features. Drug elution and deposition on the vessel wall is modeled by means of an advection-diffusion equation

and tailored boundary conditions [1]. The convective field is obtained by coupling the drug equation to a steady averaged blood flow over three heart beats; see Fig. 1. Since the healing process and drug elution span a time frame of weeks, a staggered approach is derived to simulate the drug release into the blood stream.
Advection-diffusion-reaction equations form the basis of modeling the transport and interaction of species in the vessel wall. The corresponding equations for PDGF, TGF-β, ECM and SMC can be found in [2]. The drug concentration field is coupled at the interface between the arterial wall and the lumen to account for downstream deposition of the drug. All governing equations for the wall species are coupled to a continuum mechanical description of volumetric growth.

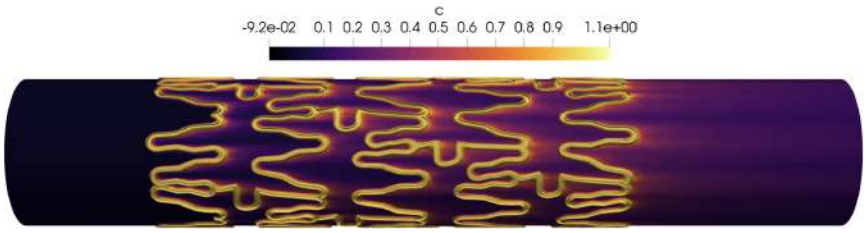


Figure 1: Drug release on artery wall with *Xience V* stent.

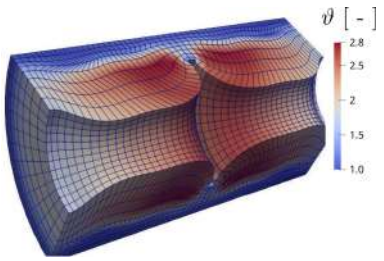


Figure 2: Growth stretch.

3 Results and conclusions

In this work we test our method on a simplified ring stent geometry with matching interface between the artery wall and the blood domain. In particular, we compare the effects of drug coupling and WSS on the endothelium and volumetric growth; see for example Fig. 2. All simulations are performed by means of finite element method using FEAP and the in-house code XNS. The aim of this work is to help provide an *in silico* tool for interventional cardiologists to tune drug-eluting stents implantation parameters.

4 Acknowledgements

Financial support of the German Research Foundation (DFG) for the project number 465213526, a subproject of the DFG priority program SPP 2311 is gratefully acknowledged.

References

[1] Hassler S, Ranno AM, Behr M. Finite-element formulation for advection–reaction equations with change of variable and discontinuity capturing. Computer Methods in Applied Mechanics and Engineering, 2020; 369: 113171.

[2] Manjunatha K, Behr M, Vogt F, Reese S. A multiphysics modeling approach for in-stent restenosis: Theoretical aspects and finite element implementation. Computers in Biology and Medicine, 2022; 150: 106166.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Finite Element Simulation of the Human Left Ventricle with Implanted Left Ventricular Assist Device: From MRI Images to a Moving Computational Domain

Maximilian Schuster[1], Norbert Hosters[1] and Marek Behr[1]

[1] Chair for Computational Analysis of Technical Systems
RWTH Aachen University, 52056 Aachen, Germany
E-mail: {schuster, hosters, behr}@cats.rwth-aachen.de, URL: www.cats.rwth-aachen.de

Key Words: *Cardiovascular Flow, Left Ventricular Assist Devices, Stabilized Finite Elements, Radial Basis Functions*

Left ventricular assist devices (LVADs) play an important role helping patients suffering from heart diseases, as they are primarily used as a bridge to transplant technology [1]. We examine the interaction between blood flow in the left ventricle (LV), LVAD, and the cannula inserted into the ventricle. We have determined stagnation and low velocity areas by solving transport equations for residence time and Virtual Ink in the ventricle under different operational conditions of the LVAD. Such areas of stagnation and low velocity are prone to thrombosis.

From a computational mechanics perspective, defining appropriate boundary conditions plays a vital role in this project for the structural and fluid mechanics part, respectively. The fluid boundary conditions at the valves, which are modelled as circular planes, progress from simple constant boundary conditions to resistance boundary conditions. They replace the circulation in the blood vessels and the flow through the LVAD whose cannula is inserted at the apex of the ventricle. The interaction between ventricle wall and fluid is imposed by the wall movement. In our current work, we make use of a magnetic resonance imaging (MRI) based LV geometry and interpolate the motion of the ventricle wall with radial basis functions. A similar approach has been presented in [2] without LVAD, thus we include the rigid body of the LVAD cannula in the computational domain. The LVAD's pump flux is set as a time-dependent Dirichlet boundary condition. The washout of blood in the LV is examined as a function of LVAD working conditions.

For the different stages of the simulations, an in-house code [3] is used. It uses a stabilized finite element method to discretize time and space. The fluid is subject to the incompressible Navier-Stokes equations with a Newtonian material law. The stagnation time as a key result of the simulations is obtained by coupling a transport equation for the residence time to the fluid equations.

REFERENCES

[1] Marsden, A.L., Bazilevs, Y., Long, C.C., Behr, M., Recent Advances in Computational Methodology for Simulation of Mechanical Circulatory Assist Devices. *Wiley Interdisciplinary Reviews: Systems Biology and Medicine,* **6** (2014) 169-188.

[2] Xu, F., & Kenjereš, S., Numerical simulations of flow patterns in the human left ventricle model with a novel dynamic mesh morphing approach based on radial basis function. *Computers in Biology and Medicine*, **130**, (2021) 104184

[3] Pauli, L., Behr, M., On Stabilized Space-Time FEM for Anisotropic Meshes: Incompressible Navier-Stokes Equations and Applications for Blood Flow in Medical Devices, *International Journal for Numerical Methods in Fluids*, **85** (2017) 189-209

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A comprehensive multiphysics mathematical model for cardiac perfusion

Zingaro Alberto[1,*], Vergara Christian[2], Dede' Luca[1], Regazzoni Francesco[1], Quarteroni Alfio[2,3]

[1] MOX, Laboratory of Modeling and Scientific Computing,
Dipartimento di Matematica, Politecnico di Milano,
Piazza Leonardo da Vinci 32, 20133, Milano, Italy

[2] LaBS, Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta",
Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133, Milano, Italy

[3] Institute of Mathematics, École Polytechnique Fédérale de Lausanne,
Station 8, Av. Piccard, CH-1015 Lausanne, Switzerland (Professor Emeritus).

Abstract: We introduce a multiphysics mathematical model to simulate the myocardial blood perfusion. Our model comprises cardiac electrophysiology, mechanics, hemodynamics, reduced valve modeling, and a multicompartment Darcy model. Specifically, we consider a fully-coupled electromechanical model [1] of the left heart that serves as unidirectional input for a fully-coupled fluid dynamics – perfusion model. In this respect, to model the blood flow in left heart (with large epicardial coronaries), we consider the Navier-Stokes equations in Arbitrary Lagrangian Eulerian framework, and we model cardiac valves by means of the Resistive Immersed Implicit Surface [2, 3] method. The fluid model is fully coupled to a three compartments Darcy model of the biventricular geometry [4]. We solve this multiphysics system by means of an implicit method with an iterative splitting strategy. We carry out simulations in the multiphysics finite element library `life`$^{\mathtt{x}}$ [5] on a realistic and geometrically detailed heart geometry. We show that our computational model can estimate coronary flow rates and myocardial blood flow maps. Furthermore, by considering then a pathological scenario, we show that the integrated model can faithfully predict the consequences of a severe aortic regurgitation in terms of a reduced myocardial perfusion.

Keywords: Cardiac modeling, Multiphysics, Cardiac Perfusion, Finite Element Method

Acknowledgements

We received funding from the Italian Ministry of University and Research (MIUR) within the PRIN (Research projects of relevant national interest 2017 "Modeling the heart across the scales: from cardiac cells to the whole organ" Grant Registration number 2017AXL54F).

References

[1] Regazzoni F., Salvador M., Africa P.C., Fedele M., Dede' L., Quarteroni A. A cardiac electromechanical model coupled with a lumped-parameter model for closed-loop blood circulation. J. Comput. Phys 2022; 457:111083.

[2] Fedele M., Faggiano E., Dede' L., Quarteroni A. A patient-specific aortic valve model based on moving resistive immersed implicit surfaces. BMMB 2017; 16:5.

[3] Zingaro, A., Fumagalli, I., Dede', L., Fedele, M., Africa, P. C., Corno, A. F., Quarteroni, A. A geometric multiscale model for the numerical simulation of blood flow in the human left heart. DCDS-S, 2022; 15:8, 2391-2427.

[4] Di Gregorio, S., Fedele, M., Pontone, G., Corno, A. F., Zunino, P., Vergara, C., Quarteroni, A. (2021). A computational model applied to myocardial perfusion in the human heart: from large coronaries to microvasculature. J. Comput. Phys, 2021; 424, 109836.

[5] Africa, P. C. `life`$^{\texttt{x}}$: a flexible, high performance library for the numerical solution of complex finite element problems. SoftwareX, 2022; 20, 101252.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Anderson acceleration for robust and scalable quasi-Newton methods

Nicolás A. Barnafi*

* Centro de Modelamiento Matemático (CMM)
Universidad de Chile
Santiago, Chile
e-mail: nbarnafi@cmm.uchile.cl

Abstract: Newton methods are usually are more expensive than other methods, despite their quadratic convergence, which has motivated the use of schemes with worse convergence but better complexity. We show how Anderson acceleration can yield tremendous improvements in solving multiphysics problems optimally with quasi-Newton methods. A careful choice of roles between which component of the problem is handled at which level (nonlinear solver, linear solver or preconditioner) is key to obtain schemes that are amenable to acceleration. The resulting schemes are, in all of our test cases, faster, more robust and present improved scalability properties than standard approaches.

Keywords: Block-partitioned solvers, non-linear methods, preconditioners, HPC.

1 Introduction

Quasi-Newton methods is nowadays a rather loose term, used to refer to any variant of a Newton method in which the Jacobian matrix is modified in order to obtain a method that converges in more iterations, but where the inversion of the (approximated) Jacobian is much easier. It is difficult *a priori* to state what is the expected rate of convergence of a given quasi-Newton scheme due to the generality of its setting. Consider the abstract root finding problem

$$F(\boldsymbol{x}) = \boldsymbol{0},$$

with a quasi-Newton scheme given by

$$\boldsymbol{B}_k \delta \boldsymbol{x}_k = -F(\boldsymbol{x}_{k-1}), \quad \boldsymbol{x}_k = \boldsymbol{x}_{k-1} + \delta \boldsymbol{x}_k.$$

In such generality, $\boldsymbol{B}_k = \boldsymbol{I}$ represents a Richardson scheme (linearly convergent, unstable), and $\boldsymbol{B}_k = \nabla F(\boldsymbol{x}_{k-1})$ represents a Newton scheme (quadratic convergence, depends on initial guess). In between there is the Broyden family, with superlinear convergence, and even Uzawa schemes for saddle point problems, which represent a Richardson iteration for the Schur complement. Still, in all cases, such iterative methods can be represented by the fixed-point iteration

$$\boldsymbol{x}_k = g(\boldsymbol{x}_{k-1}),$$

which can be accelerated using Anderson acceleration [1]. However, it has been recently proved that Anderson acceleration can accelerate linearly converging sequences, but not necessarily quadratically convergent ones, as it induces second order error terms [2]. This means, for instance, that a Newton scheme cannot be accelerated, at least not with this technique.

2 Methodology

We leverage the convergence theory of Anderson acceleration to relax the Newton method until an iteration that can be accelerated is obtained. Suppose that the Jacobian matrix is difficult to precondition and can be split into into matrices, one which can be preconditioned optimally, and the difference:

$$\nabla F(\boldsymbol{x}_k) = \boldsymbol{A}_k + \boldsymbol{R}_k, \quad \boldsymbol{R}_k := \nabla F(\boldsymbol{x}_k) - \boldsymbol{A}_k$$

This induces a quasi-Newton scheme given by

$$\boldsymbol{A}_k \delta \boldsymbol{x}_k = -F(\boldsymbol{x}_{k-1}),$$

which will probably lose the quadratic convergence of the Newton scheme, but each iteration can be solved optimally. The loss of quadratic convergence can then be alleviated with Anderson acceleration, which grants robustness to the nonlinear scheme. The resulting scheme is better understood as an accelerated Richardson scheme, preconditioned by the action of the inverse of the approximate Jacobian. This highlights that the action of the inverse in most cases might not be exact, and could be approximated simply by the action of the preconditioner, which allows us to completely circumvent the use of an Krylov iteration at the Jacobian level. We have validated this approach in many different scenarios, such as fluid dynamics and poroelasticity, where the resulting scheme is notoriously more robust and scalable than standard approaches.

3 Acknowledgements

This work has been partially funded by the Proyecto Basal FB210005, as well as the chilean National Laboratory of HPC (NLHPC).

References

[1] Walker H, Ni P. Anderson acceleration for fixed-point iterations. SIAM Journal on Numerical Analysis, 2011;49.4:1715-1735.

[2] Evans C, Pollock S, Rebholz LG, Xiao M. A proof that Anderson acceleration improves the convergence rate in linearly converging fixed-point methods (but not in those converging quadratically). SIAM Journal on Numerical Analysis, 2020;58.1:788-810.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Boundary integral formulation and numerical experiments on the Cell-by-Cell model for electrophysiology

Giacomo Rosilho de Souza[*], **Simone Pezzuto**[*†] **and Rolf Krause**[*]

[*] Center for Computational Medicine in Cardiology, Euler Institute, Università della Svizzera Italiana,
via G. Buffi 13, 6900 Lugano, Switzerland
e-mail: {giacomo.rosilhodesouza,rolf.krause}@usi.ch

[†] Department of Mathematics, Università di Trento,
via Sommarive 14, 38123 Povo (Trento), Italy
e-mail: simone.pezzuto@unitn.it

Abstract: The cell-by-cell model for cardiac electrophysiology, also called Extracellular-Membrane-Intracellular (EMI) model, describes the evolution of electric potentials at the cellular level, specifically: within each cell, in the extra-cellular space and on the transmembrane boundary. These models are degenerate parabolic equations, consisting of elliptic equations in the intra- and extra-cellular domains, the intercellular coupling conditions, and a time dependent membrane model on the transmembrane boundary. Employing a boundary-integral formulation, we recast the problem to a non degenerate parabolic equation on the transmembrane boundary, where the differential operator is nonlocal. In particular, we show that the spatial discretization of the cell-by-cell model leads to an ordinary differential equation on the transmembrane boundary. Then, we present some numerical experiments where we: asses the efficiency and accuracy of the numerical discretization and study how model parameters as the cells size, gap junctions distribution, and conductivities affect the action potential conduction velocity.

Keywords: Electrophysiology, Cell-by-Cell Model, EMI model, Boundary Element Method.

1 Introduction

We consider the prototypical cell-by-cell model

$$\begin{cases} -\sigma_i \Delta u_i = 0, & \text{in } \Omega_\mathrm{i} \text{ for } i = 1, \dots, N, & \text{(1a)} \\ -\sigma_e \Delta u_e = 0, & \text{in } \Omega_\mathrm{e}, & \text{(1b)} \\ -\sigma_i \partial_{\boldsymbol{n}_i} u_i = C_\mathrm{m} \dfrac{\mathrm{d}V_\mathrm{m}}{\mathrm{d}t} + I_\mathrm{ion}(V_\mathrm{m}, z) & \text{on } \Gamma_{im} \text{ for } 1 \le i \le N, & \text{(1c)} \\ -\sigma_e \partial_{\boldsymbol{n}_e} u_e = -C_\mathrm{m} \dfrac{\mathrm{d}V_\mathrm{m}}{\mathrm{d}t} - I_\mathrm{ion}(V_\mathrm{m}, z), & \text{on } \Gamma_m, & \text{(1d)} \\ -\sigma_e \partial_{\boldsymbol{n}_e} u_e = 0, & \text{on } \Sigma, & \text{(1e)} \\ u_i - u_e = V_\mathrm{m}, & \text{on } \Gamma_{im} \text{ for } 1 \le i \le N, & \text{(1f)} \\ \dfrac{\mathrm{d}z}{\mathrm{d}t} = g(V_\mathrm{m}, z), & \text{on } \Gamma_m, & \text{(1g)} \\ -\sigma_i \partial_{\boldsymbol{n}_i} u_i = \kappa(u_i - u_j) & \text{on } \Gamma_{ij} \text{ for } 1 \le i, j \le N. & \text{(1h)} \end{cases}$$

In (1), the transmembrane potential V_m depends on the ionic model I_ion, z, g and as well on the extra- and intra-cellular potentials u_e and u_i, $i = 1, \dots, N$, where N is the number of cells. Cells are defined by the intra-cellular domains Ω_i and Ω_e is the extra-cellular domain, while

σ_i, σ_e are cell conductivities and κ is the intercellular permeability constant. Intercellular connections happen at the intersections $\Gamma_{ij} = \partial\Omega_i \cap \partial\Omega_j$ between two distinct cells. The transmembrane boundary is $\Gamma_m = \cup_{i=1}^{N} \Gamma_{mi}$, with $\Gamma_{mi} = \partial\Omega_e \cap \partial\Omega_i$, and $\Sigma = \partial\Omega_e \setminus \Gamma_m$ is the outer boundary. The normals $\boldsymbol{n}_i$, $\boldsymbol{n}_e$ point outwards to Ω_i, Ω_e, respectively.

Model (1) has been solved by the finite element method in, for instance, [3]. The boundary element method (BEM) has been employed in [1], however only for simple settings of non touching cells, hence without condition (1h). Recently, in [2], we propose a BEM approach for problems with touching cells.

2 Spatio-temporal discretization

In [2] we recast problem (1) into a boundary integral formulation and employ a collocation based BEM for its spatial discretization. This procedure yields an ordinary differential equation confined on the transmembrane boundary Γ_m, hence where the temporal dynamics takes place (see (1c) and (1d)). This result is summarized in Theorem 1.

Theorem 1. *The BEM space discretization of* (1) *is equivalent to the ordinary differential equations system*

$$\begin{cases} C_m \dfrac{\mathrm{d}\boldsymbol{V}_m}{\mathrm{d}t} + I_{ion}(\boldsymbol{V}_m, \boldsymbol{z}) = \psi(\boldsymbol{V}_m), & \text{(2a)} \\ \dfrac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}t} = g(\boldsymbol{V}_m, \boldsymbol{z}), & \text{(2b)} \end{cases}$$

where $\psi : \mathbb{R}^{M_m} \to \mathbb{R}^{M_m}$ *is a self-adjoint linear map and* M_m *is the number of nodes lying on* Γ_m.

In (2) we recover a reaction-diffusion model with a nonlocal diffusion operator ψ encoding the elliptic equations (1a) and (1b), the intercellular conditions (1f) and (1h), the boundary condition (1e), and flux continuity. Equation (2) closely resembles the monodomain equation, routinely solved in the cardiac electrophysiology community.

Acknowledgements This work was supported by the European High-Performance Computing Joint Undertaking EuroHPC under grant agreement No 955495 (MICROCARD) co-funded by the Horizon 2020 programme of the European Union (EU) and the Swiss State Secretariat for Education, Research and Innovation.

References

[1] Henríquez, F., Jerez-Hanckes, C.: Multiple traces formulation and semi-implicit scheme for modelling biological cells under electrical stimulation. ESAIM: Mathematical Modelling and Numerical Analysis **52**, 659–702 (2018)

[2] Rosilho de Souza, G., Pezzuto, S., Krause, R.: Boundary integral formulation of the cell-by-cell model of cardiac electrophysiology (in preparation) (2022)

[3] Tveito, A., Mardal, K.A., Rognes, M.E.: Modeling Excitable Tissue: The EMI Framework. Springer Nature (2021)

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Scalable BDDC preconditioners for hybrid DG discretizations of cardiac microscopic models

Huynh, Ngoc Mai Monica*

* Dipartimento di Matematica
Università degli Studi di Pavia
Pavia, Italia
e-mail: ngocmaimonica.huynh@unipv.it

Abstract: In this talk we will give an insight of a Balancing Domain Decomposition by Constraints (BDDC) preconditioner for Discontinuous Galerkin discretizations of cardiac cell-by-cell models in order to approximate the discontinuous nature of cellular networks and the associated electrical potentials. These recent mathematical models are based on individual representation of cardiac cells and provide a detailed description of the multiscale structure and dynamics of the heart, overcoming some of the limitation of the homogenized macroscopic cardiac Bidomain and Monodomain models. The resulting discrete cell-by-cell models have discontinuous global solutions across the cell boundaries, hence the proposed BDDC preconditioner is based on appropriate dual and primal spaces with additional constraints which transfer information between cells (subdomains) without influencing the overall discontinuity of the global solution. Our theoretical convergence rate analysis shows scalability and quasi-optimality of the proposed BDDC preconditioned cell-by-cell operator. These theoretical bounds are then validated through extensive numerical tests, further confirming scalability, quasi-optimality, and independence from the time step size of the BDDC preconditioner.

Keywords: Domain decomposition preconditioners, BDDC, discontinuous Galerkin, cardiac cell-by-cell models

1 Short abstract

Recent mathematical models of cardiac functions provide a detailed description of the multiscale structure and dynamics of the heart, based on microscopic cardiac cell-by-cell models, recently introduced in order to overcome some of the limitations of the macroscopic Bidomain and Monodomain models, where cell membrane, intracellular and extracellular spaces coexist at each point of the cardiac tissue. While this assumption has played a key-role in the development and the increase of interest in computational cardiology field, it does not allow for a microscopic representation of the tissue.

However, cell-by-cell models based on individual representation of cardiac cells allow for instance for realistic modeling of damaged tissue and for studying the effects of nonuniform distributions of ion channels on the cell membrane. Generally, these models consider the aforementioned objects (cell membrane, intra and extracellular spaces) in a coupled manner, allowing for discontinuous potentials across the boundaries of cells as well as general representations in terms of geometries.

The numerical simulation of these complex cardiac models is very challenging since it requires high-resolution space and time discretizations, as well as numerical tools that can handle

natural discontinuities, arising for instance between different cells.

In this talk we will give an insight of a Balancing Domain Decomposition by Constraints (BDDC) preconditioner for Discontinuous Galerkin discretizations of cell-by-cell models in order to approximate the discontinuous nature of cellular networks and the associated electrical potentials.

The resulting discrete cell-by-cell models have discontinuous global solutions across the cell boundaries, hence the proposed BDDC preconditioner is based on appropriate dual and primal spaces with additional constraints which transfer information between cells (subdomains) without influencing the overall discontinuity of the global solution.

Our theoretical convergence rate analysis shows scalability and quasi-optimality of the proposed BDDC preconditioned cell-by-cell operator. These theoretical bounds are then validated through extensive numerical tests, further confirming scalability, quasi-optimality, and independence from the time step size of the BDDC preconditioner.

References

[1] Huynh NMM, Chegini F, Pavarino LF, Weiser M and Scacchi S. Convergence analysis of BDDC preconditioners for hybrid DG discretizations of the cardiac cell-by-cell model. ArXiv preprint arXiv:2212.12295 (2022).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Monolythic coupling of a viscoelastic surface and a viscous fluid

de Kinkelder Eloy*, Aland Sebastian†

* Istitute for numerical mathematics and optimisation
Institut für numerische Mathematik und Optimierung, Technische Bergakademie Freiberg
Freiberg, Germany
e-mail: eloymerlijn.dekinkelder@htw-dresden.de

† Istitute for numerical mathematics and optimisation
Institut für numerische Mathematik und Optimierung, Technische Bergakademie Freiberg
Freiberg, Germany
e-mail: Sebastian.Aland@math.tu-freiberg.de

Abstract: Viscoelastic surface rheology plays an important role in multiphase systems. A typical example is the actin cortex which surrounds most animal cells. It shows elastic properties for short time scales and behaves viscous for longer time scales. Hence, realistic simulations of cell shape dynamics require a model capturing the entire elastic to viscous spectrum. We model the cell cortex as a viscoelastic surface suspended in a 3-dimensional viscous fluid. For this we use the surface equivalent of the upper convected Maxwell model, also distinguishing between shear and areal stresses. The surface is suspended in a viscous fluid, modelled by the Stokes equation. To couple both system we use an Arbitrary Lagrange-Eulerian method. Initially, the forces generated by the surface were set explicitly as boundary conditions in the fluid. This however, results in a harsh time step restriction for dominantly viscous surfaces. So to avoid this, a monolythic coupling is implemented, allowing us to solve the fluid structure interaction as one system. This implementation will allow us to solve a larger variety of problems.

Keywords: Viscoelastic, cell cortex, finite elements, Stokes, ALE

1 Introduction

The cell cortex is a thin cross-linked network of the polymerised protein actin. It underpins the membrane surrounding animal cells. The cortex is a key regulator for the emergence of cell shape and is vital for cell function, for instance during cell division. On short time scales (< 1 s) the cortex exhibits a dominantly elastic in-plane response to external mechanical stresses. On larger time scales (> 10 s) the cortex can undergo dynamic remodelling because of network rearrangement which results in a fluid-like rheology. So to capture both properties, a viscoelastic implementation is needed [1]. In [2] a numerical model for a viscoelastic surface embedded in a viscous fluid is proposed. To model the viscoelasticity, a surface equivalent of the upper convected Maxwell model is constructed. For the numerical implementation the finite elements method is used. The surface and the bulk are coupled using an Arbitrary Lagrangian-Eulerian method (ALE). Both systems are solved separately, the forces generated by the surface are used as boundary conditions for the fluid equations. This however, resulted in a harsh time step restriction when these forces contain spatial derivatives, as is the case with a viscous surface. To circumvent this, we propose a monolythic coupling of the surface and bulk equations. This allows us to solve the system of equations as one, removing the time step restriction.

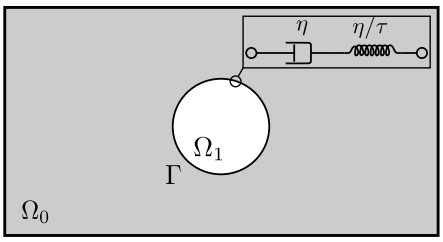


Figure 1: A 2-dimensional sketch of the domain. Internal fluid Ω_1, external fluid Ω_0 separated by the surface Γ. The surface is viscoelastic with viscosity η and elastic modulus η/τ, where τ is the relaxation time. In the actual model we distinguish between shear and areal viscosities and relaxation times.

2 Extended abstract content

Our model consists of three domains, two 3-dimensional domains for the internal and external fluid and one 2-dimensional surface representing the cell cortex (Fig. 1). Due to the low Reynolds number, the fluid is modelled by the Stokes equations. For the viscoelastic surface we use the surface equivalent of the upper convected Maxwell model as defined in [2]. The stress S is split into the shear and areal stress. The areal stress is represented by $\mathrm{tr}S$ and the shear stress by the traceless stress tensor $\bar{S} = S - \frac{\mathrm{tr}(S)}{2}P$. Here P is the projection matrix, which projects vectors on the surface Γ. The equations expressing the viscoelastic dynamics are,

$$\bar{S} = 2\eta_S \bar{D}_\Gamma - \tau_S \overset{\nabla}{\oint}_t \bar{S} + (\boldsymbol{v}\cdot\nabla_\Gamma)\bar{S} - \nabla_\Gamma \boldsymbol{v}_\Gamma \bar{S} - \bar{S}(\nabla_\Gamma \boldsymbol{v}_\Gamma)^T + P(\bar{S} : \nabla_\Gamma \boldsymbol{v}_\Gamma) - \mathrm{tr}(S)\bar{D}_\Gamma.\big) \qquad \text{on } \Gamma, \quad (1)$$

$$\mathrm{tr}(S) = 2\eta_A \mathrm{tr}(D_\Gamma) + \tau_A \overset{\nabla}{\oint}_t (\bar{S} : \nabla_\Gamma \boldsymbol{v}_\Gamma) + \mathrm{tr}(S)\mathrm{tr}(D_\Gamma) - \partial_t^\bullet \mathrm{tr}(S) - (\boldsymbol{v}\cdot\nabla_\Gamma)\mathrm{tr}(S)\big) \qquad \text{on } \Gamma. \quad (2)$$

Here $\boldsymbol{v}$ is the velocity, D_Γ is the surface rate of deformation and $\bar{D}_\Gamma$ its trace less version. The differential operator ∇_Γ projects the derivatives on the surface using the projection matrix P. The parameters are the shear and areal viscosities η_S, η_A and the relaxation times τ_S, τ_A. To couple the surface and the bulk equations the following boundary condition on the surface Γ is used,

$$\nabla_\Gamma \cdot S = \big[-pI + \eta_i \overset{\nabla}{\oint} \nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)\big]_0^1 \cdot \boldsymbol{n} \qquad \text{on } \Gamma. \quad (3)$$

The angular brackets represent the jump in value across the surface Γ, p is the pressure, $\boldsymbol{n}$ is the normal of Γ and the parameter η_i is the viscosity of the fluid on the domain Ω_i.

3 Conclusions

Implementing the described model with an explicit coupling between the surface and the bulk equations results in a harsh time step restriction. This makes it impossible to simulate cases with dominant spatial derivatives on the surface. With a monolythic coupling this time step restriction disappears.

References

[1] M. Mokbel, K. Hosseini, S. Aland, and E. Fischer-Friedrich. The Poisson Ratio of the Cellular Actin Cortex Is Frequency Dependent. Biophys. J. 2020;118.8; 1968–1976

[2] de Kinkelder E, Sagis L, Aland S. A numerical method for the simulation of viscoelastic fluid surfaces. J. Comput. Phys. 2021; 440; 110413.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Neural Networks as spectral approximators in evolution problems involving several time-scales. Application to glioblastoma progression.

Jacobo Ayensa-Jiménez[1], Marina Pérez-Aliacar[1] and Manuel Doblaré[1]

[1] Aragon Institute of Engineering Research (I3A)
Universidad de Zaragoza, Spain

e-mail: jacoboaj@unizar.es

Abstract: Artificial Neural Networks are used as Reduced-Order Models in many dynamical problems involving separated time-scales for accelerating computations. However, their discrete nature makes them impractical for many applications due to the curse of dimensionality. We present here a framework where ANNs are used as functional surrogates in the low scale dynamics. Good representations are obtained with very few variables using spectral approximations which reduces the computational cost at the fast scale to an inner product computation. The method is applied to hypoxia-mediated glioblastoma progression, where two different time scales (oxygen diffusion and cell migration) have a dynamical interplay, illustrating that accurate enough solutions may be obtained with much less computational cost.

Keywords: Spectral methods, Multiscale problems, Artificial Neural Networks.

1. INTRODUCTION

Simulation of evolution problems involving different time scales is challenging and computationally demanding [1]. Among the existing methods for facing these problems, Reduced-Order Models (ROM) are a good alternative for obtaining accurate representations at the low time-scale impacting the high-scale dynamics. Artificial Neural Networks (ANN) are nowadays extensively used in many contexts as ROMs thanks to their expressivity. However, ANNs have a discrete nature and suffer the curse of dimensionality for representing discrete numerical simulations. Our aim is to use the spectral coefficients of the different involved fields (for instance using Legendre polynomials) as their representation to feed the different ANNs. One dynamical system where two different time-scales are involved is glioblastoma (GBM) progression in hypoxic conditions, where fast dynamics (oxygen diffusion) interplays with low dynamics (cell migration) [2]. GBM is the most common and deadly primary brain tumor and hypoxia seems to play an important role in its progression. We evaluate the method performance for simulating the evolution of GBM.

2. METHODS

We split the fast and slow dynamics of the problem in two flow operators $\mathfrak{F}^\tau$ and $\mathfrak{G}^\tau$ depending on a marching step τ that are evaluated consecutively. The functional map $\boldsymbol{\mathfrak{F}^\tau}: \boldsymbol{\mathcal{C}^\infty(I)} \rightarrow \boldsymbol{\mathcal{C}^\infty(I)}$, $\boldsymbol{\mathfrak{F}^\tau(u) = v}$, is represented by $\boldsymbol{F}: \mathbb{R}^{\boldsymbol{n}} \rightarrow \mathbb{R}^{\boldsymbol{n}}$, $\boldsymbol{F(u) = v}$, where $\sum_i \boldsymbol{u_i \phi_i}$ and $\sum_i \boldsymbol{v_i \phi_i}$ are truncated spectral representations of $\boldsymbol{u}$ and $\boldsymbol{v}$. The fast scale operator $\boldsymbol{\mathfrak{F}^\tau}$ is expressed as $\boldsymbol{\mathfrak{F}^\tau(u)} \simeq \sum_{i=1}^{n} \boldsymbol{F_i(u) \phi_i}$, where $\boldsymbol{u} = (\boldsymbol{u_1}, \dots, \boldsymbol{u_n})$. To build the representation $\boldsymbol{F}$, we use the expressiveness of ANNs. The network can be trained using high-fidelity simulation data or the residual of the PDE as a loss function.

The proposed method is applied to a biological problem of interest, as it is GBM progression in hypoxic conditions. The cell concentration is represented by a field $u = u(x, t)$, whose dimensionless evolution equation is:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(P\frac{\partial u}{\partial x} - \chi u f(v)\frac{\partial v}{\partial x}\right) + \alpha g(v)u(1-u), \tag{2}$$

where P, χ and α are model parameters related with cell pedesis, chemotaxis and growth, respectively, and $v = v(x,t)$ is the oxygen concentration. The functions f and g are activation functions that account for the role of hypoxia in cell migration and death. The oxygen field follows another evolution equation:

$$\frac{\partial v}{\partial t} = D\frac{\partial^2 v}{\partial x^2} - \frac{\beta v}{v+1}u, \tag{3}$$

where D and β are also model parameters. Cell migration time-scale is of the order P^{-1} wereas oxygen diffusion time-scale is of the order D^{-1}. As usually $P \ll D$ and Eqs. (1) and (2) are coupled, so GBM evolution is an example multiscale evolution problem.

3. RESULTS

The approximation capacity of the methodology is illustrated in Figure. 1, where the solutions obtained using numerical simulation are compared to the ones obtained by ANNs and spectral approximation, for four slow scale solutions. A speed-up factor of 50±10 is obtained while keeping a relative L_2 error of (3±1)‰ for 100 different samples.

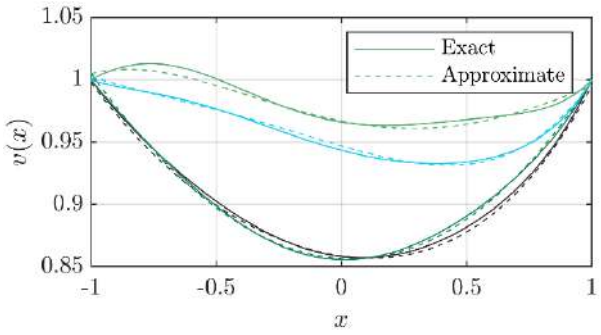


Figure 1. Exacted and approximated solutions for four different slow scale solutions.

4. CONCLUSIONS

The combination of spectral representations with ANNs is able to accurately approximate solutions of partial differential equations modelling evolution systems. This enables the use of this technique for addressing dynamical problems with separated time-scales.

Acknowledgements

The author gratefully acknowledge the financial support from the Spanish Ministry of Science and Innovation (MICINN through the project PID2021-126051OB-C41.

References

[1] Kuehn, C. Multiple time scale dynamics (2015). Springer..

[2] Ayensa-Jiménez, J. et al. (2020). Mathematical formulation and parametric analysis of in vitro cell models in microfluidic devices: application to different stages of glioblastoma evolution. Scientific Reports, 10(1), 21193.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Development of New Surgical Mesh Geometries with Different Mechanical Properties Using the Design Freedom of 3D Printing

Sterk Sebastian[*], Silva M.E.T.[†] Fernandes A.A. [†]

[*] Faculty of Engineering
University of applied Sciences Frankfurt, Frankfurt, Germany
e-mail: sebastian.sterk@stud.fra-uas.de

[†] Faculty of Engineering
Universidade do Porto, Porto, Portugal
e-mail: mesilva@inegi.up.pt

[†] Faculty of Engineering
Universidade do Porto,Porto, Portugal
e-mail: aaf@fe.up.pt

Abstract: The use of various rapid prototyping technologies in connection with the development of new medical products offers a newfound freedom of shape design that allows direct influence on the mechanical properties. Meltelectrowriting offers the possibility to redesign surgical meshes and their geometry, creating different geometries with different mechanical properties without changing the material. The adaptation of the mechanical properties plays an important role in the transplantation of medical products into a host tissue in order to imitate the mechanical behavior of the host tissue as well as possible. For this purpose, a large number of single wavy fibres and wavy fibre meshes were designed and printed using an optimised printing process to mimic the mechanical behaviour of collagen. The mechanical examination of the printed fibres and meshes combined with statistical experimental design methods shows a widely varying behavior that can imitate the most diverse host tissues as elastic soft tissues with mesh deformations up to 100% elongation and a Young´s Modulus ranging from 100 to 400 MPa. A adaptation of the geometry to the soft tissue of the human vaginal wall shows a sufficient fitting and can be improved by further adjustments of the geometry.

Keywords: melt electrowriting; surgical mesh; pelvic organ prolapse; polycaprolactone; rapid prototyping

1. Introduction

The high complication rate of meshes for Pelvic Organ Prolapse (POP) shows the relevance of improved meshes related to their materials and structure. The research in this work focuses on improving the meshes by using modern technologies in rapid prototyping as meltelectrowriting (MEW) to produce ultrafine polymer structures that should mimic the biomechanical properties of vaginal tissue and find suitable materials for surgical meshes. It is assumed that the complex structure of the pelvic floor and the non-specific meshes with a structure not adapted to the pelvic floor are responsible as the main reason for the high error rate in surgical meshes [1,2]. For better compatibility, the surgical meshes will be made of biodegradable polymers, which are already widely used in medicine [3]. The surgical meshes are designed to mimic the mechanical behavior of the human vaginal wall.

2. Materials and Methods

The fibres and meshes are based on the wave-like structure of collagen fibres, which on the one hand ensures the elastic behaviour of the fibres and meshes and on the other hand leads to an auxetic behaviour of the meshes. The waves of the fibres and meshes differ in their amplitude and number of waves per total length of the fibres. The mathematical description of these waves enables the path-controlled creation of G-codes with FullControl [4]. A uniaxial testing machine (MultiTest-i, Mecmesin GmbH, Freiburg, Germany) with a clamping system is used to examinate the test. The force is determined with a 10N Loadcell. All tests carried out follow the same test protocol. The sample geometry is 35x10 mm strips for printed meshes and for single fibres 35 mm in length. The samples are clamped in their original stress-free state and stretched at a rate of 10 mm/min until failure.

3. Results

Figure 1a shows the stress-strain behaviour for wavy fibres. The stress-strain curve can be divided into 3 zones (toe region, linear region and yield point). The fibres differ in their yield strength, yield strain, toe region and young's modulus. For sinusoidal meshes, we obtain a stress-strain curve for a uniaxial tensile test, which is very similar to the stress-strain curves of single wavy fibres and collagen fibres (Figure 1b). Even in the mesh composite, the wavy fibres retain their mechanical properties and resemble soft tissues in their stress-strain behaviour. The fibre geometry has a significant influence on the mechanical properties of the mesh and can be specifically controlled to mimic the mechanical behaviour of prolapsed vaginal tissue (Figure 1c) [5].

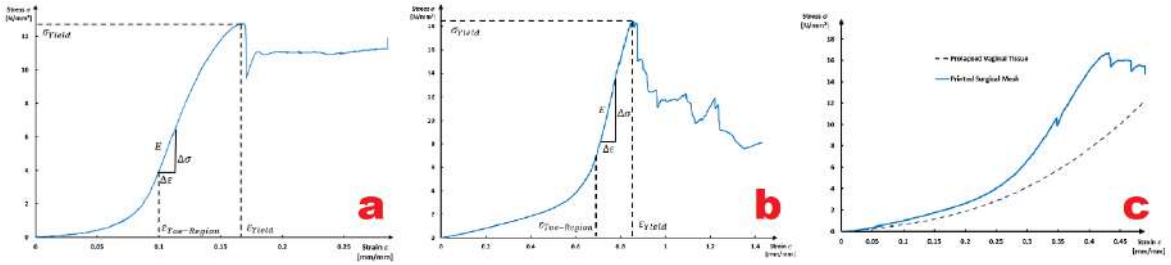


Figure 1a) Stress-Strain curve for uniaxial test on single wavy fibres b) Stress-Strain curves for uniaxial test on wavy meshes c) Stress-Strain curve for printed wavy mesh and prolapsed vaginal tissue [5]

4. Conclusions

The preceding investigations show that the mechanical properties of printed fibres depend significantly on their geometry. The printing parameters only play a subordinate role when it comes to influencing the mechanical properties. In the uniaxial tensile test, wavy fibres strongly resemble the behaviour of soft tissues and collagen fibres in particular. By changing the amplitude and the number of waves per total length of the fibre, the mechanical behaviour of the fibre can be controlled. The displacement of the toe region and the elastic behaviour are decisive. The behaviour of a single fibre can also be transferred to fibre composites in the form of a mesh. If vertical and horizontal fibres are only connected at nodes and do not overlap, the mechanical properties in the vertical and horizontal directions are largely independent for uniaxial tensile tests. A superposition of horizontal and vertical waves leads to a mixing of the mechanical properties in the horizontal and vertical direction, which leads to a blurring of the toe region and worsens the reproducibility of the mechanical behaviour. Due to the large mechanical range covered by the meshes due to their different geometries, a good imitation of different soft tissues can be achieved by a controlled design of the fibre and thus of the mesh. This range can be significantly extended by using different plastics.

References

[1] Rynkevic, Rita, June 2019, In vivo models and in silico simulations of mesh augmented prolapse repair, Faculty of Engineering University of Porto, Porto
[2] Mironska, E., Chapple, C., & MacNeil, S. (2019, June 4). Recent advances in pelvic floor repair. F1000Research.
[3] New advancements of bioplastics in medical applications: International Journal of Pharmaceutical Sciences and Research. IJPSR. (2021, December 27).
[4] https://fullcontrolgcode.com/
[5] Calvo, B., Peña, E., Martins, P., Mascarenhas, T., Doblaré, M., Jorge, R. M. N., & Ferreira, A. (2009, January 21). On modelling damage process in vaginal tissue. Journal of Biomechanics.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A machine learning-based prediction of pelvic floor stress during vaginal delivery

Rita Moura*†, Dulce Oliveira†, Marco Parente†, Renato Natal Jorge†

† INEGI-LAETA, Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: up201404216@edu.fe.up.pt, doliveira@inegi.up.pt, mparente@fe.up.pt, rnatal@fe.up.pt

Abstract: The second stage of labor is commonly associated with childbirth trauma. To better understand and quantify this phenomenon, finite element models are often utilized. However, models can be quite demanding in terms of computational resources. To mitigate this issue, machine learning (ML) techniques have been used to predict simulation outcomes. A pre-trained ML algorithm can significantly reduce the time required to obtain the desired results. The present study aims to predict urogenital hiatus stresses using material properties of the pelvic floor as inputs. A dataset was generated using data from 2189 finite element simulations, and various ML models were tested. Hyperparameter tuning with cross-validation was also implemented. The results revealed a mean absolute error of 0.627 with the Extreme Gradient Boosting model and 0.564 with Neural Networks. This work represents a preliminary approach to predict the outcome of childbirth simulations through the use of ML techniques. The results suggest that this approach may apply to more complex problems. Predicting stresses or other relevant biomechanical indicators based on specific material properties of the tissue could aid in clinical decision-making.

Keywords: Childbirth simulations, Finite element method, Machine learning, Real-time biomechanics

1 Introduction

The second stage of labor is associated with obstetric trauma during labor, leading to long-term consequences such as incontinence and prolapse. These conditions greatly impact a woman's quality of life [1]. Computational models and the finite element method (FEM) are commonly used to analyze the mechanics of labor. However, these complex simulations require substantial amounts of time to yield desired results. Recently, researchers in the biomechanical field have been recurring to machine learning (ML) algorithms to reduce the time and cost of simulations [2]. This work aims to use ML models to predict the stresses on key regions of the pelvic floor muscles (PFM) during vaginal delivery, using different input material parameters to characterize these muscles.

2 Methodology

A dataset was created using FEM simulations of childbirth with different Martins constitutive model (Equation 1) material properties to characterize the PFM [3].

$$U = c\{e^{b\left(\bar{I}_1^C - 3\right)} - 1\} + A\{e^{[a(\bar{\lambda}_f - 1)^2]} - 1\} \tag{1}$$

The c, b and A material constants varied in specific ranges, whereas a was kept constant. A

total of 2189 simulations were successfully completed. A dataset was created in which each node of the pelvic floor corresponds to an observation. A total of 50 nodes of the PFM near the urogenital hiatus were selected, resulting in a total of 109450 observations. Features such as simulation number, node number and position, initial coordinates, and material parameters were used for training. Five models, namely Decision Trees (DT), Random Forest (RF), Extreme Gradient Boosting (XGBT), Support Vector Regression (SVR), and Neural Networks (NN), were chosen for the study. A training and test set were created with a 90/10 split, followed by hyperparameter optimization with cross-validation. The models' performance was measured by the mean squared error and the mean absolute error.

3 Results

In the FEM simulations, the stresses of the urogenital hiatus varied between approximately 0 and 50 kPa, thus ML models must predict values within this range.

Preliminary results of the tested algorithms are presented in Table 1. Performance assessment demonstrated that XGBT and Neural Networks provided the best results.

Table 1: Mean squared error (MSE) and mean absolute error (MAE) obtained for the ML algorithms used.

	DT	**RF**	**XGBT**	**SVR**	**NN**
MSE	12.172	12.172	0.974	8.896	**0.812**
MAE	2.605	2.605	0.627	1.783	**0.564**

4 Conclusions

This study uses FEM childbirth simulation data to train ML algorithms for near real-time predictions. The results obtained are promising and can be further optimized by gathering additional data and use of alternative methods to increase the models' performance. In a clinical setting, identifying stress levels or other relevant indicators in the pelvic floor can provide a patient-specific biomechanical analysis of potential delivery issues.

5 Acknowledgements

The authors gratefully acknowledge the support from Portuguese Foundation of Science under the Grant SFRH/BD/05876/2021, the Junior Researcher Contract CEECIND/01522/2020, and the funding of Project UIDB/50022/2020.

References

[1] Doumouchtsis, S. Childbirth Trauma. Springer, 2016

[2] Phellan R, Hachem B, Clin J, Duong L. Real-time biomechanics using the finite element method and machine learning: Review and perspective. Med. Phys. 2021.

[3] Martins JAC, Pires EB, Salvado E, Dinis PB, A numerical model of passive and active behavior of skeletal muscles. Comput Methods Appl Mech Eng, 1998.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Biomechanics of the fetal membrane as a multilayer biological structure

Fidalgo Daniel[*], Oyen Michelle[†], Oliveira Dulce[*], Parente Marco[*], Natal Renato[*], Myers Kristin[††]

[*] Instituto de Ciência e Inovação em Engenharia Mecânica e Engenharia Industrial (INEGI)
Porto, Portugal
e-mail: dfidalgo@inegi.up.pt, doliveira@inegi.up.pt, mparente@up.pt, rnatal@up.pt

[†] McKelvey School of Engineering
Washington University
Washington, United States
e-mail: oyen@wustl.edu

[††] Department of Mechanical Engineering
Columbia University in The City of New York
New York, United States
e-mail: kmm2233@cumc.columbia.edu

Abstract: The fetal membrane is an essential biological structure to protect the fetus. Its multilayer structure (amnion, chorion, and part of the decidua) and its microstructure will dictate the mechanical behavior of the membrane throughout the gestational period. Resorting to the potential of numerical simulation, this work aims to access fetal membrane biomechanics, highlighting the importance of its multilayer nature.

Keywords: Fetal Membrane; Amnion; Chorion; Constitutive Model; Numerical Simulation.

1. Introduction

The fetal membrane is a complex biological structure that surrounds and protects the fetus, [1]. It is a multilayered structure, comprising the amnion, the chorion, and part of the decidua. It undergoes complex microstructural changes by the end of pregnancy [2], which will contribute to the weakening of the tissue in preparation for delivery [3]. Several factors associated with the mechanical response and the microstructure of the fetal membrane remain unknown and few studies were performed to define an accurate constitutive model able to characterize its mechanics. This work aimed to analyze the biomechanics of the fetal membrane resorting to the finite element method.

2. Methodology

The inflation experimental data used to calibrate the multiplayer model was obtained by the *Skala Lab* - Morgridge Institute for Research. The calibration was performed by adjusting the numerical apex displacement of our finite element numerical inflation setup to the experimental apex displacement reported by the *Skala Lab*. In terms of constitutive models, the amnion was characterized by the modified version of the Buerzle-Mazza constitutive model (μ_o=2.4MPa, q=2.96, m5=0.463, m2=0.00228, m3=41.12, m4=1.27, N=32, v=0), whose properties were retrieved from the literature, except for μ_o, which was obtained from inverse finite element analysis. The chorion (E=1MPa, υ=0.41) and the decidua (E=1MPa, υ=0.49) were characterized by elastic linear properties. The simulation of the inflation mechanical test was performed according to the protocol followed by the Skala Lab. The maximum principal stresses were analyzed in the amnion and the chorion layers.

3. Results

Figure 1 (left) illustrates the maximum principal stress distribution in the amnion and chorion layers at the end of the inflation simulation. The graphic represented in Figure 1 (right) shows the maximum principal stress evolution throughout the inflation test at the apex region of each fetal membrane layer. According to Figure 1, at the end of the mechanical test, the amnion layer exhibits a maximum principal stress value of 4156 kPa at the apex region, while the chorion only exhibits a value of 219 kPa. Focusing on the graphic, it is also important to highlight that the amnion is submitted to much higher stresses than the chorion throughout the entire mechanical simulation of the inflation test, highlight the mechanical dominance of the amnion.

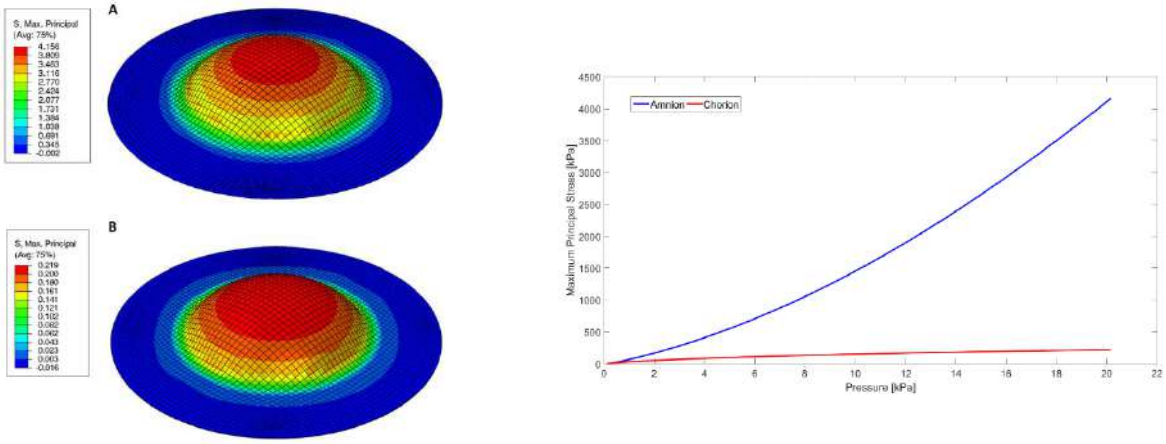


Figure 1. (Left) Maximum principal distribution in the amnion (A) and chorion (B) layers at the end of the simulation of the inflation mechanical test (units: MPa). (Right) Maximum principal stress evolution in the amnion and chorion layers throughout the simulation of the inflation mechanical test.

4. Conclusions

A multilayer fetal membrane model able to capture its mechanical behavior was developed and calibrated. To do so, a brand-new dataset was used, obtaining a great fit between the numerical and the experimental outcomes. Besides that, the overall behavior of the amnion and the chorion are also consistent with previous numerical and experimental works [4].

References

[1] Jabareen, M., Mallik, A.S., Bilic, G., Zisch, A.H., Mazza, E., 2009. Relation between mechanical properties and microstructure of human fetal membranes: an attempt towards a quantitative analysis. Eur. J. Obstet. Gynecol. Reprod. Biol. 144 Suppl, 134–141.

[2] McLaren, J., Malak, T.M., Bell, S.C., 1999. Structural characteristics of term human fetal membranes prior to labour: Identification of an area of altered morphology overlying the cervix. Hum. Reprod. 14, 237–241.

[3] Oyen, M.L., Calvin, S.E., Landers, D. V., 2006. Premature rupture of the fetal membranes: Is the amnion the major determinant? Am. J. Obstet. Gynecol. 195, 510–515.

[4] Verbruggen, S.W., Oyen, M.L., Phillips, A.T.M., Nowlan, N.C., 2017. Function and failure of the fetal membrane: Modelling the mechanics of the chorion and Amnion. PLoS One 12, 1–14.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

The inverse FEM analysis for the estimation of biomechanical properties of the continent and incontinent woman bladder

Agostinho Pedro[1], Silva Elisabete[2], Brandão Sofia[3], Mascarenha Teresa[4], Fernandes António[1]

[1]LAETA, INEGI, Faculty of Engineering, University of Porto, Porto, Portugal
email: up202001582@edu.fe.up.pt; aaf@fe.up.pt

[2]LAETA, INEGI, Porto, Portugal
email: mesilva@inegi.up.pt

[3]Department of Radiology, Centro Hospitalar de São João-EPE, Faculty of Medicine, University of Porto, Porto, Portugal
email: sofia.brand@gmail.com

[4]Department of Gynecology and Obstetrics, Centro Hospitalar de São João-EPE, Faculty of Medicine, University of Porto, Porto, Portugal
email:tqc@sapo.pt

Abstract: The female pelvic cavity is a very complex anatomical region. Pelvic dysfunction, especially pelvic organ prolapse (POP) and urinary incontinence (UI), have a negative impact on women's lives, and it happens when the support mechanisms of the pelvic cavity become fragile. Existing treatments for these disorders are divided into conservative and invasive. The last ones consist of surgical interventions and should be used in patients in whom the first treatments did not work, or when the severity of the dysfunction is high.
This study focuses on adapting an inverse finite element analysis (FEA) to estimate the *in vivo* properties of the bladder, using a constitutive model of the female pelvic cavity and magnetic reso-nance images acquired at rest and during the Valsalva maneuver, for two disctint groups (continent and incontinent women). The bladder neck's displacements were compared between computational simulation and magnetic resonance images.
The results of the FEA showed that the bladder tissue of incontinent women have the highest stiffness approximately 47% higher when compared to continent women.
Keywords: Bladder; Stress Urinary Incontinence; Intra-abdominal pressure; Material Parameters; Inverse Finite Element Analysis

1. Introduction

Urinary incontinence (UI) has a prevalence of a up to 28%, with stress urinary incontinence (SUI) being the most common form [1], [2], characterized by involuntary urinary leakage during physical strain, coughing or an increase in intra-abdominal pressure (IAP). Assessment of bladder neck (BN) mobility in patients with SUI is essentially clinical, however, the imaging techniques such as ultrasound (US) and magnetic resonance imaging (MRI) are used as a method for evaluating this characteristic. The outcomes of radiographic images have been crucial and used as input for numerical methods.The aim of the present study was to establish the IAP values and the *in vivo* biomechanical properties of the bladder tissue for two distinct groups (continent women and women with SUI). The numerical simulations of Valsalva maneuver were performed, applying the Ogden hyperelastic constitutive model to the bladder and also the inverse finite element analysis (FEA).

2. Material and Methods

this work, in order to evaluate the presence and symptoms of UI, a cohort of 11 women (n=6, Continent (control group) and n=5 with UI) was recruited and submitted to scanning magnetic resonance imaging. In order to obtain the IAP and *in vivo* biomechanical properties of the bladder in the two distinct groups (continent group (CG) and incontinent group (IG)),

it was adapted a 3D computational model (Figure 1A)) of the female pelvic cavity [3], that corresponds a nulliparous 24 years old healthy female.

A) B)

Figure 1. A) Computational model of the female pelvic cavity. B) Bladder and pelvic support structures impaired for the IG.

3. Results

Figure 2 presents the results of the mechanical response of the uniaxial stress-stretch response for the 2 groups to compare the effect of material parameters (Table 4) obtained in this work, compared with the experimental curve.

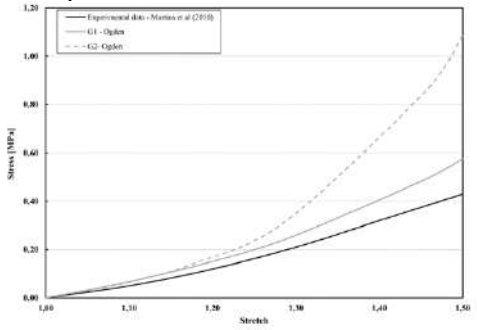


Figure 2. Uniaxial stress–stretch response for behaviour of the bladder for the Ogden constitutive model and experimental data of the literature.

4. Conclusions

The biomechanical properties for the bladder of the Ogden constitutive model from the CG and IG have a difference of approximately 47% in stiffness, being greater for IG.

Acknowledgements

The authors gratefully acknowledge funding from Stimulus of Scientific Employment 2021.00077.CEECIND, financed through FCT. This work was supported by FCT, through INEGI, under LAETA, project UIDB/50022/2020 and UIDP/50022/2020.

References

[1] M. H. Jansson, K. Franzén, G. Tegerstedt, A. Hiyoshi, and K. Nilsson, “Stress and urgency urinary incontinence one year after a first birth—prevalence and risk factors. A prospective cohort study,” *Acta Obstet. Gynecol. Scand.*, vol. 100, no. 12, pp. 2193–2201, 2021, doi: 10.1111/aogs.14275.

[2] K. Falah-Hassani, J. Reeves, R. Shiri, D. Hickling, and L. McLean, “The pathophysiology of stress urinary incontinence: a systematic review and meta-analysis,” *Int. Urogynecol. J.*, vol. 32, no. 3, pp. 501–552, 2021, doi: 10.1007/s00192-020-04622-9.

[3] S. Brandão *et al.*, “On the Stiffness of the Mesh and Urethral Mobility: A Finite Element Analysis,” *J. Biomech. Eng.*, vol. 139, no. 8, pp. 1–9, 2017, doi: 10.1115/1.4036606.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A finite element analysis of breast compression in mammography

Carvalho Mariana[1,2], **Arduino Alessandro**[3], **Parente Marco**[1,2], **Natal Jorge Renato**[1,2], **Ferreira João**[1]

[1] Department of Mechanical Engineering (DEMec)
Faculty of Engineering, University of Porto
Porto, Portugal

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

[3] Department of Civil, Environmental, and Architectural Engineering
University of Padova
Padova, Italy

Abstract: Cancer remains a critical health concern despite multiple advances towards early diagnosis and alternative treatments. Breast cancer is the most common neoplasia among adult women. Early detection using imaging techniques, such as x-ray mammography, can increase the patient's prognosis and 5-year survival rate. X-ray mammography employs breast compression to obtain a 2D image. Biomechanical models of the breast can assist clinicians with physics-based approaches to address critical health scenarios. In this work, a biomechanical breast model is presented to serve as a platform for studies on breast biomechanics. The *in-silico* model includes the geometric and material definition of different breast structures: ribs, pectoralis muscle, fibroglandular and fat tissues and skin. To prove its applicability, a finite element analysis of a craniocaudal mammography setup is employed with displacement control. Taking glandularity levels from 5 to 60% and a 50 mm compressed breast thickness (CBT), the measured compression force of 100 to 140 N is within the range of clinical measurements reported in de Groot (2015) for the same CBT and breast volume.

Keywords: breast, mammography, large deformations, finite element analysis.

1. INTRODUCTION

Breast cancer is the most incident and the leading cause of death from cancer in adult women globally [1]. X-ray mammography is the gold standard for breast cancer's early detection and diagnosis. This technique flattens the breast between two paddles to obtain a 2D x-ray projection. Higher compression levels provide a more uniform compressed breast thickness (CBT) and improve the differentiation between tumours and normal tissue. In clinical practice, the ability to employ large compression levels depends on factors such as breast density, size and volume and the patient's pain resistance [2]. This work focuses on developing a general breast biomechanical model to be subjected to significant compression levels characteristic of a mammographic exam.

2. Materials and methods

The biomechanical model, with a breast volume between 0.20 and 0.52 dm^3 [3], is composed of linear elastic ribs, pectoralis muscle and skin and hyperelastic isotropic adipose and fibro-glandular tissues described by a Mooney-Rivlin formulation. Breast glandularity is ranged between 5 and 60% (Figure 1). The skin is meshed by shell elements and a hexahedral structured mesh is applied to the remaining geometries. The rib bones are locked without any degree of freedom and tied constraints restrict the relative motion between contacting surfaces. A quasi-static finite analysis of a craniocaudal (CC) compression is performed in

Abaqus Explicit (Figure 1). The breast model is placed between rigid analytical paddles with symmetric displacements. A frictionless contact is defined at the breast-paddles interface.

Figure 1. CC compression (a) with illustration of the different layers for 5% (b) and 60% (c) glandularity.

3. Results and discussion

The material models and properties used enabled a realistic breast deformation, as the in-plane geometry enlarged by paddle compression. Additionally, the maximum principal stress in the skin is maximum at the contact point near the ribs (Figure 2). For a 50 mm-CBT, the compression force ranges from 100 to 140 N (for higher glandularity levels) which approaches clinical measurements [3] for the same CBT and breast volume.

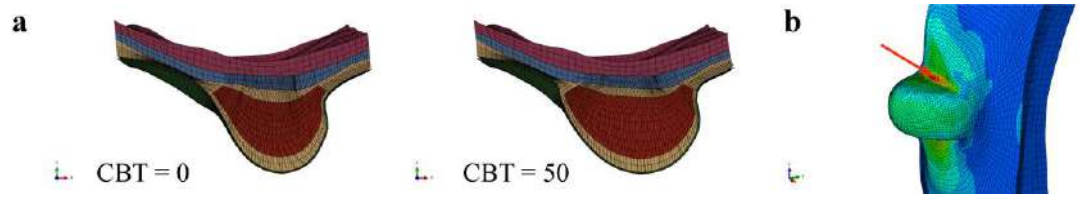


Figure 2. Breast deformation (a) and maximum stress distribution (arrow points to the maximum value) (b).

4. Conclusions

The model produced can accommodate large breast compressions characteristic of a mammography examination. Although not based on real mammogram setups, the obtained force approaches clinical results. Future works should include breast tumours.

Acknowledgments

The authors gratefully acknowledge the support from the Portuguese Foundation of Science under grant SFRH/BD/09480/2022 and the funding of project PTDC/EME-APL/1342/2020.

References

[1] Sung H, Ferlay J, Siegel RL, Laversanne M, Soerjomataram I, Jemal A, et al. Global Cancer Statistics 2020: GLOBOCAN Estimates of Incidence and Mortality Worldwide for 36 Cancers in 185 Countries. CA Cancer J Clin 2021;71:209–49.

[2] Babarenda Gamage TP, Nielsen PMF, Nash MP. Clinical Applications of Breast Biomechanics. Biomechanics of Living Organs: Hyperelastic Constitutive Laws for Finite Element Modeling 2017:215–42.

[3] de Groot JE, Broeders MJ, Grimbergen CA, den Heeten GJ. Pain-preventing strategies in mammography: an observational study of simultaneously recorded pain and breast mechanics throughout the entire breast compression cycle. BMC Womens Health 2015;15:26.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Mathematical and numerical modeling of axonal beading

D. Riccobelli

MOX – Dipartimento di Matematica
Politecnico di Milano
Milan, Italy
e-mail: davide.riccobelli@polimi.it

Abstract: Many neurodegenerative diseases and pathologies (e.g. viral infections, Parkinson's and Alzheimer's diseases) can damage neurons by destroying the microtubule cytoskeleton. Such a physical damage can modify the morphology of axons leading to axonal beading, i.e. the formation of sequences of bulges along the axon. In this talk, we present a mathematical model of axonal beading based on the theory of continuum mechanics. Axons are described as nonlinear elastic cylinders coated with an elastic layer representing the actomyosin cortex. Such a cortex is in active tension thanks to the action of myosin II motors. We show that axonal beading is the result of an elastic instability induced by the coupling of cortex contractility and microtubule depolymerization. We also discuss the numerical implementation of the nonlinear boundary value problem. We propose a discretization based on the finite element method, where we use a parameter continuation algorithm to compute the bifurcation diagram.

Keywords: Axon, buckling, FEM, bifurcation, mechanobiology

1 Introduction

In this talk, we present a mathematical and numerical model of axonal beading, namely the formation of sequences of bulges. Such shape changes can be induced by Parkinson's and Alzheimer's diseases, multiple sclerosis, viral infections, and many other pathologies. Several experimental evidences show that such a morphological degeneration is correlated with a reduction of the number of microtubules in axons [2].

2 Mathematical modelling

We describe the axon as a continuum medium, composed of an inner part, called axoplasm, and a tubular coating, which represents the actomyosin cortex. The reference configuration of the axon is a cylinder $\Omega = \{\boldsymbol{X} \in \mathbb{E}^3 \mid \|\boldsymbol{X}\| < R_o\}$, while $\boldsymbol{\varphi} : \Omega \to \mathbb{E}^3$ is the deformation field. We denote by $\mathsf{F} = \operatorname{Grad} \boldsymbol{\varphi}$ the deformation gradient.

The active contraction of the cortex is modeled by means of the active strain approach: the deformation gradient is decomposed into an active and an elastic contribution [3, 1]:

$$\mathsf{F} = \mathsf{F}_\mathrm{e}\mathsf{F}_\mathrm{a}.$$

Both the axoplasm and the cortex are assumed to be incompressible and to behave as neo-Hookean material with different shear moduli, indicated with μ_a and μ_c, respectively.

The stability of the cylindrical physiological configuration is analyzed through the method of incremental deformations. By fixing the active stretch of the cortex and the thickness of

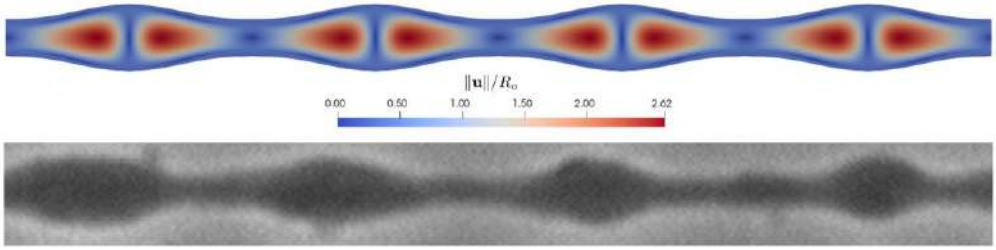


Figure 1: Top: predicted morphology of a buckled axon (adapted from [3]). Bottom: beaded neurite after exposure to Nocodazole (adapted from [2]).

the actin cortex, we find the critical stiffness ratio $\mu = \mu_c/\mu_a$ for which a bifurcation takes place and the corresponding wavenumber. Thus, axonal beading can be described as the buckling of the axon induced by cytoskeleton damage and cortex contractility.

2.1 Numerical simulations

The post-buckling behaviour of the damaged axon is investigated by using numerical simulations. The nonlinear boundary value problem is discretized by using the mixed finite element method. The computational domain corresponds to an axial section of the axon and we use a triangular mesh. The displacement and the pressure fields are approximated by using $\boldsymbol{P}_2 - P_0$ elements, ensuring that the inf-sup condition is satisfied. In order to track the bifurcation diagram, a small perturbation is applied to the mesh and we exploit a simple natural parameter continuation algorithm. The numerical scheme is implemented using the open-source library FEniCS.

The outcomes of the numerical simulations are in perfect agreement with the theoretical predictions of the stability analysis and qualitatively reproduce the experimental results, see Fig. 1.

3 Acknowledgements

This work has been supported by National Group of Mathematical Physics (GNFM – INdAM) through the program *Progetto Giovani* and by Regione Lombardia project NEWMED (Grant No. POR FESR 2014-2020).

References

[1] Andrini D, Balbi V, Bevilacqua G, Lucci G, Pozzi G, Riccobelli D. Mathematical modelling of axonal cortex contractility. Brain Multiphysics 2022;3:100060.

[2] Datar A, Ameeramja J, Bhat A, Srivastava R, Mishra A, Bernal R, Prost J, Callan-Jones A, Pullarkat, PA. The roles of microtubules and membrane tension in axonal beading, retraction, and atrophy. Biophys J 2019;117(5):880-891.

[3] Riccobelli D. Active elasticity drives the formation of periodic beading in damaged axons. Phys Rev E 2021;104(2):024417.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Interictal Spike Propagation Reconstruction in the Epileptic Brain: Mapping with Invasive versus Noninvasive Techniques

Margherita A.G. Matarrese[*,†,‡], **Eleonora Tamilia**[§], **M Scott Perry**[†], **Alessandro Loppini**[*], **Joseph R. Madsen**[§], **Steve M. Stufflebeam**[‖], **Phillip L. Pearl**[§], **Simonetta Filippi**[*], **Christos Papadelis**[†,‡,‡]

[*] Unit of Non-Linear Physics and Mathematical Modeling, Engineering Department, Università Campus Bio-Medico di Roma, Rome, Italy
(e-mail to: m.matarrese@unicampus.it)

[†] Jane and John Justin Institute for Mind Health Neurosciences Center, Cook Children's Health Care System, Fort Worth, TX, USA

[‡] Department of Bioengineering, The University of Texas at Arlington, Arlington, TX, USA

[§] Boston Children's Hospital, Harvard Medical School, Boston, MA, USA

[‖] Athinoula A. Martinos Center for Biomedical Imaging, Massachusetts General Hospital, Harvard Medical School, Boston, MA

[‡] School of Medicine, Texas Christian University, Forth Wort, TX, USA.

Abstract: Spikes are a key epilepsy biomarker showing a propagating phenomenon across large brain areas. The ability of different techniques, such as invasive EEG, HD-EEG, and MEG, to capture the same phenomenon is currently unexplored. Here, we aim to delineate the spatiotemporal propagation of spikes noninvasively and compare it with the invasive phenomenon. We analyzed iEEG, HD-EEG, and MEG data from 4 children with drug-refractory epilepsy who underwent resective neurosurgery with good surgical outcome (Engel 1). For each patient, we reconstructed the spike propagation in the source domain with wMEM across the different modalities and evaluated the similarities and differences between the propagations recorded with the different techniques.

Keywords: Source Imaging, Spike propagation, Epilepsy Biomarkers, Inverse Problem

1. Introduction

Interictal spikes are frequent and brief, high-amplitude waveforms that can be recorded with both noninvasive (i.e., HD-EEG and MEG) and invasive techniques (iEEG). Most patients with epilepsy (~90%) show spikes, and several studies have reported spike propagating phenomena across the cortex. Indeed, spikes do not occur in a single contact each time, but they are detected by multiple contacts at a time with a specific spatial displacement and temporal duration [1]. These phenomena can be tracked on the cortical surface with high temporal and spatial accuracy with electric and magnetic source imaging, providing useful clinical information regarding the underlying pathophysiology of such events [2]. Here, we aim to assess the spike propagation variability intra- and across modalities (i.e. HD-EEG, MEG and iEEG) in pediatric patients with drug-refractory epilepsy (DRE).

2. Materials and Methods

We retrospectively analyzed interictal intracranial EEG (iEEG) data and simultaneous HD-EEG and MEG recordings from 4 children with DRE who had successful (Engel 1, 1 year after surgery) resective neurosurgery at Boston Children's Hospital. For each modality, interictal spike propagations were visually detected and spatiotemporally reconstructed in the source domain with Wavelet Maximum Entropy on the Mean (wMEM) [3]. We used

the Desikan-Killiany cortical parcellation to identify the anatomical gyrus involved across the propagations at a specific time frame. We computed the duration, the total displacement and the speed of each spike propagation. Finally, for each modality, we obtained a patient-specific map representing the most recurrent active area(s) involved in the propagation.

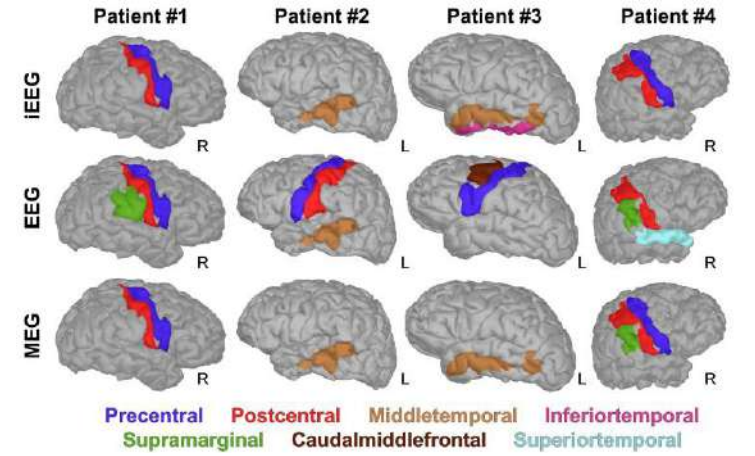


Figure 1. Patient-specific maps of recurrent spike regions across modalities. Each color is a specific gyrus in the cortical surface.

3. Results

We detected a total of 318 spikes propagations for iEEG, 202 for HD-EEG and 317 for MEG in 5 minutes of clean recordings. We found no difference in the spike propagation duration between modalities (iEEG: 40 ms [20-60 ms]; HD-EEG: 35 ms [15-75 ms]; MEG: 30 ms [15-75 ms]; $p>0.5$) and no difference in the spatial displacement between iEEG and MEG (iEEG: 2 cm [1-4 cm]; HD-EEG: 4 cm [1-8 cm]; MEG: 2 cm [1-5 cm]). However, the HD-EEG showed higher spatial displacement than iEEG ($p<0.001$) and MEG ($p<0.001$) and the highest velocity of propagation (iEEG: 0.5 m/s [0.3-0.9 m/s]; HD-EEG: 1.0 m/s [0.5-1.5 m/s]; MEG: 0.6 m/s [0.4-1.0 m/s]). The patient-specific spike maps for each modality are shown in Figure 1. Considering the iEEG as the gold standard, the MEG was always concordant with the iEEG, while the HD-EEG was concordant in 3 patients out of 4 and involved more areas than the iEEG.

4. Conclusions

In this study, we provide, for the first time, a comparison between spike propagation mapping in invasive and noninvasive modalities, showing that noninvasive techniques may localize the same phenomenon recorded invasively. To better understand this phenomenon, further investigation is needed to confirm these findings on a wider population.

Acknowledgments

This work was supported by the National Institute of Neurological Disorders & Stroke (RO1NS104116-01A1, PI: C. Papadelis), and Cook Children's Health Foundation. M.A.G. Matarrese, A. Loppini and S. Filippi acknowledge the support of the National Group for Mathematical Physics (GNFM-INdAM).

References

[1] G. Alarcon *et al.*, "Origin and propagation of interictal discharges in the acute electrocorticogram. Implications for pathophysiology and surgical treatment of temporal lobe epilepsy," *Brain*, vol. 120, no. 12, pp. 2259–2282, 1997, doi: 10.1093/brain/120.12.2259.

[2] N. Tanaka *et al.*, "Propagation of epileptic spikes reconstructed from spatiotemporal magnetoencephalographic and electroencephalographic source analysis," *Neuroimage*, vol. 50, no. 1, pp. 217–222, Mar. 2010, doi: 10.1016/j.neuroimage.2009.12.033.

[3] J. M. Lina, R. Chowdhury, E. Lemay, E. Kobayashi, and C. Grova, "Wavelet-based localization of oscillatory sources from magnetoencephalography data," *IEEE Trans Biomed Eng*, vol. 61, no. 8, pp. 2350–2364, 2014, doi: 10.1109/TBME.2012.2189883.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Flow of cerebrospinal fluid in cranial subarachnoid space: a mathematical model

Dvoriashyna Mariia and Goriely Alain

Mathematical Institute
University of Oxford
Oxford, United Kingdom
e-mail: dvoriashyna@maths.ox.ac.uk, goriely@maths.ox.ac.uk

Abstract: Cerebrospinal fluid (CSF) is a clear, transparent fluid that bathes the brain and spinal cord. It fills the subarachnoid space (SAS), which surrounds the spinal canal and the brain and is exteriorly lined by the dura membrane. During the cardiac cycle, this fluid pulsates following the time varying changes of brain volume. In this work, we study oscillatory and steady streaming CSF flow in cranial SAS in order to understand its role in solute transport in SAS and waste clearance. We develop a theoretical model of the flow using lubrication theory. The model suggests that steady streaming plays an important role in solute transport.

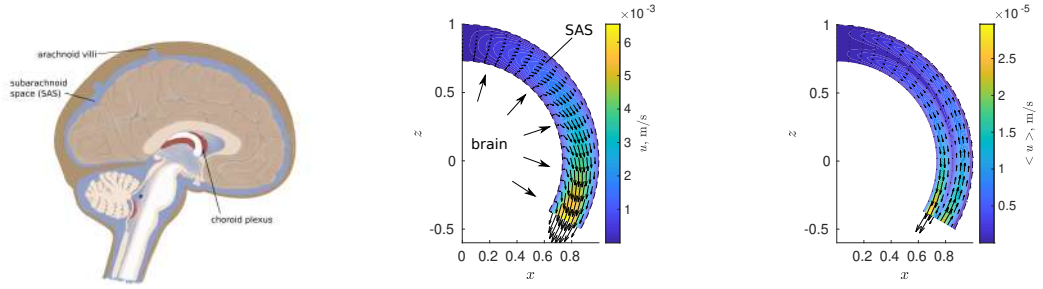
Keywords: cerebrospinal fluid, lubrication theory, cerebral fluid mechanics

1 Introduction

Cerebrospinal fluid (CSF) is a clear, transparent fluid with water-like properties. It is produced mainly in the choroid plexus, at a rate of 25mL/hour, it flows through ventricles into the subarachnoid space (SAS), which is a fibrous space that covers spinal cord and the brain and it is exteriorly lined by the dura membrane (see Figure 1a). The fluid is then drained through arachnoid villi into the saggital sinus, located at the top of the head. Apart from the slow production-drainage flow, there is also a pulsating flow in SAS driven by arterial pulsation: during systole, CSF flows from the cranial to the spinal SAS, and during diastole, the flow reverses [1]. One of the roles of this flow is to contribute to the transport and clearance of metabolic waste from the brain. Several studies have addressed CSF flow in both spinal (*e.g.* analytical and numerical works [3, 4, 2]) and cranial SAS (*e.g.* numerical studies of [5]). To complement existing numerical works, in this study we investigate flow in cranial SAS using an analytical technique, lubrication theory.

2 Methods and Results

We model the SAS in spherical coordinates as a region between two radial surfaces $R_1(\theta, \phi, t) \leq r \leq R_2(\theta, \phi)$, with $0 \leq \theta \leq \theta_0$ and $0 \leq \phi \leq 2\pi$, which are separated by thickness $h = R_2 - R_1$. h oscillates periodically, following prescribed brain displacements during cardiac cycle. We neglect the presence of the fibres in SAS and model the flow with Navier-Stokes equations for incompressible fluid. We simplify these equations using lubrication theory since the aspect ratio of the domain is small. We also expand the solution as a Fourier series in time, which allows us to obtain a second-order equation for the pressure for each time harmonic.



(a) (b) (c)

Figure 1: (a) Drawing of the cross section of the human brain. (b) Flow at the right half of the brain for $h = h(t)$, at an instant when brain expands. (c) Steady streaming flow. The r coordinate and component of the flow are magnified by a factor of 20 for better visualisation.

For the simplified case of a spherical brain surface and spatially uniform thickness h, we obtain the analytical solution shown in Figure 1b. As a result of these oscillations, there is a steady streaming flow (Figure 1c). In the case of non-uniform thickness h, we obtain complex three-dimensional flow fields with velocities of about 10^{-5} m/s, which are comparable to the magnitude of production-drainage flow.

3 Conclusions

We developed and solved a model of CSF flow in cranial SAS with the use of lubrication theory. We find that steady streaming flow caused by oscillations is comparable to production-drainage flow in SAS and thus contributes to the transport of solutes.

4 Acknowledgements

The support by the Engineering and Physical Sciences Research Council of Great Britain under research grant no. EP/R020205/1 to A.G. is gratefully acknowledged.

References

[1] Miller K. Biomechanics of the Brain. Springer; 2011.

[2] Linninger AA, *et al.* Cerebrospinal fluid mechanics and its coupling to cerebrovascular dynamics. Annual Review of Fluid Mechanics. 2016; 48:219-57.

[3] Sanchez AL, *et al.* On the bulk motion of the cerebrospinal fluid in the spinal canal. Journal of Fluid Mechanics. 2018; 841:203-27.

[4] Salerno L, Cardillo G, Camporeale C. Aris-Taylor dispersion in the subarachnoid space. Physical Review Fluids. 2020;5(4):043102.

[5] Gupta S, *et al.* Cerebrospinal fluid dynamics in the human cranial subarachnoid space: an overlooked mediator of cerebral disease. I. Computational model. Journal of the Royal Society Interface. 2010; 7(49):1195-204.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Uncertainty quantification and control of kinetic models of tumour growth with uncertain features

Andrea Medaglia

Department of Mathematics, University of Pavia, Pavia, Italy
e-mail: andrea.medaglia02@universitadipavia.it

Abstract: We propose a kinetic model of tumour growth considering the effects of clinical uncertainties. Therapeutic protocols aiming at reducing the tumour's volume are constructed by means of selective-type controls that affect the cellular dynamics. By using statistical mechanics tools for many-agent systems, we find that it is possible to reduce clinical uncertainties across scales. To account for the lack of clinical data and potential errors in image segmentation, we calibrate the model using real cases of primary glioblastoma and then we reconstruct the empirical distributions. In the end, we discuss suitable numerical methods for uncertainty quantification in the resulting kinetic equations and we compare the effectiveness of the control approaches in reducing the variability in tumour's size caused by the uncertain quantities.

Keywords: kinetic modelling; tumour growth; uncertainty quantification; optimal control

1 Introduction

Uncertainty is a fundamental aspect of physical, biological, and socio-economical systems, and should be considered in the corresponding mathematical models, formulated through partial differential equations (PDEs), to provide a more data-oriented representation of these phenomena. This uncertainty can be either *epistemic*, arising from incomplete knowledge of the system, or *aleatoric*, intrinsic to the system and that cannot be reduced through measurements. From a mathematical viewpoint, these uncertain quantities are considered as random variables $\mathbf{z} \in \mathbb{R}^{d_\mathbf{z}}$, with $d_\mathbf{z} \in \mathbb{N}$, affecting the dynamics and increasing automatically the dimensionality of the PDEs, and leading to the well-known *curse of dimensionality*.

This is a particularly interesting problem in the kinetic framework: kinetic equations have been recently employed to mimic the emergence of collective phenomena in life sciences, see [3, 4] and the references therein. One of the main challenges in utilizing the classical toolset of kinetic theory for these systems is the absence of first principles that define the microscopic dynamics. Together with the lack of accurate experimental results for many collective phenomena, this means that uncertainty is naturally embedded into the models, and the parameters are described only as statistical information. Therefore, the study of these problems requires the construction of numerical methods that preserve the structure of the equations and the asymptotic state, which is often unknown. In addition, the analysis of real data and the calibration of parameters are very important aspects for extracting quantitative information about models.

2 Modelling and control of tumour growth under clinical uncertainties

In [2], we develop a kinetic model of tumour growth taking into account the effects of clinical uncertainties affecting the tumours' progression. The time variation of the distribution function is due to the elementary transitions occurring at the cellular level, taking environmental cues and random fluctuations into account [4]. In suitable limits, the expected cellular variations are coherent with well-known ODE-based models, i.e., the Gompertz and the von-Bertalanffy models. The emerging distributions of the kinetic model in the presence of uncertain quantities show slightly different behaviour: Gompertz-type growth is linked to slim-tailed distributions, while von-Bertalanffy-type growth is associated with fat-tailed distributions connected to a higher probability that the tumours' volume is non-negligible.

In order to mimic the action of therapeutic protocols trying to reduce the tumours' volume, suitable robust selective-type controls acting at the level of cellular dynamics have been implemented. This control setting is based on Boltzmann-type controls in which an optimal control problem is solved at the microscopic level and then analysed at the mesoscopic scale using the classical multi-scale methods of kinetic theory. In this framework, the analytical characteristics of the asymptotic regime are analysed and it is demonstrated that the introduced control, acting at the cellular level, is able to dampen the structural uncertainties at the macroscopic/observable level.

Hence, thanks to a close collaboration with IRCCS Mondino Foundation of Pavia we estimate the real impact of uncertain quantities in the developed model on a dataset for primary glioblastoma. The introduction of uncertain parameters results in the previously discussed increase of dimensionality of the resulting kinetic problem, whose equilibrium depends on all the uncertainties introduced at the cellular level.

In this direction, several lines of research can be developed. First of all, to estimate the parameters and design effective control strategies it may be interesting to further investigate nonconvex optimization, which has proven to be effective for agent-based models since typically the resulting minimization problem does not have a single global minimum but rather a number of local minima. Besides, as proposed in [1], uncertainties in the parameter defining the growth-type model may provide more accurate results with respect to data.

References

[1] Franceschi J, Medaglia A, Zanella M. On the optimal control of kinetic epidemic models with uncertain social features. arXiv preprint 2022; arXiv:2210.09201.

[2] Medaglia A, Colelli G, Farina L, Bacila A, Bini P, Marchioni E, Figini S, Pichiecchio A, Zanella M. Uncertainty quantification and control of kinetic models of tumour growth under clinical uncertainties. Int. J. Non Linear Mech. 2022; 141:103933.

[3] Pareschi L, Toscani G. Interacting multiagent systems: kinetic equations and Monte Carlo methods. OUP Oxford; 2013.

[4] Preziosi L, Toscani G, Zanella M. Control of tumor growth distributions through kinetic methods. J. Theor. Biol. 2021;514:110579.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A Quantitative Systems Pharmacology approach to drive mRNA-vaccine design

Fiandaca Giada[*], Zangani Natascia[*], Leonardelli Lorena[†], Giampiccolo Stefano[†], Selvaggio Gianluca[†] and Marchetti Luca[*,†]

[*] Department of Cellular, Computational and Integrative Biology (CIBIO)
University of Trento
Trento, Italy

[†] Fondazione the Microsoft Research
University of Trento Centre for Computational and Systems Biology
Rovereto, Italy

Abstract: In this talk, we present a Quantitative Systems Pharmacology (QSP) model to simulate the mRNA vaccine-induced immunogenicity to investigate its efficacy and to support its optimization in terms of formulation, dose and schedule finding. The resulting simulations consistently reproduce the early events that follow an mRNA-based vaccination in both innate and humoral response, considering product specific, cell specific and tissue specific properties.

Keywords: mRNA-vaccine, dose and schedule finding, Quantitative Systems Pharmacology (QSP), mathematical modeling, computational tools, drug development support

1 Introduction

At the outset of the COVID-19 pandemic, the need increasingly emerged for an efficient vaccination methodology, ensuring a sufficient immunogenic response as well as prompt supply, large dose availability and low production cost. Among all proposed methods, mRNA-vaccines proved to be good candidates in this direction: they guarantee rapid and scalable production, while the cell's translation machinery ensures proper protein folding and post-translation modifications. Unfortunately, as of the early 2020, there was only limited clinical experience with this technology; in particular, no systematic procedure existed to optimize vaccine-induced immunogenicity, leading to a heterogeneous scenario of vaccination strategies. To address this issue, several clinical studies are currently taking place worldwide, to evaluate the efficacy of mRNA-vaccines over time, against both the primitive and emerging virus variants, investigating the different immunogenic response observed among individuals. An impelling future challenge is to promptly design vaccine formulations and to optimize dosing and scheduling to best exploit the responsivity of this technology; thus, an in-depth understanding of the processes driving mRNA vaccine-induced immunogenicity may contribute to accelerating in silico its development and optimization.

2 Methods

Mathematical models and computational tools can play a crucial role in supporting best-candidate selection. Their ability to simulate virtual populations can indeed be pivotal in

exploring non-standard designs, and in informing vaccine formulations, dose and schedule finding, thus eventually minimizing attrition rates. To this aim we here present a QSP (Quantitative Systems Pharmacology) approach to model the main events following the administration of an mRNA-vaccine, focusing on the immunogenic response. The immunogenicity development is described at organism level and depends on vaccine type, doses and delivery systems. In accordance with the intrinsic multiscale nature of the phenomenon, a molecular layer is also included to account for mRNA specific properties, potentially providing a prototype capable of simulating different scenarios tailored to product specifics. The model extends the one presented in [1], to describe in greater detail the early events after vaccine injection for an mRNA-based formulation. It is based on information retrieved in literature through a text-mining procedure, to shift its design and development towards a knowledge-oriented approach [2]. The model is defined as a system of ODEs (Ordinary Differential Equations) that represent the whole immunogenic process, providing as endpoint to the simulation the generated antibody titers [3], and it is calibrated on literature data [4]. The embedded molecular layer is also defined in terms of ODEs, and it represents the starting phase of an mRNA-based vaccination, i.e., the presentation of the mRNA-encoded antigen by the Antigen Presenting Cells that fuel the immunogenic response.

3 Conclusions

The main tunable properties of the vaccine have been identified, and a corresponding sensitivity analysis has been carried out to suggest ways to rank drug design strategies, and to inform drug development. The resulting simulations recapitulate the main aspects of mRNA vaccine-derived immunogenicity. They consistently reproduce the early events that follow an mRNA-based vaccination in both innate and humoral response, considering product specific, cell specific and tissue specific properties. Moreover, they show how in silico tools can be employed as instruments to compare different optimization strategies, in terms of both dose and schedule finding, in the drug development process from the early discovery stage [5].

References

[1] X. Chen et al., A mechanistic, multiscale mathematical model of immunogenicity for therapeutic proteins: part-1 theoretical model, CPT: Pharmacometrics and Systems Pharmacology, 3.9: 1-9, 2014.

[2] L. Leonardelli et al., Literature mining and mechanistic graphical modelling to improve mRNA vaccine platforms, Frontiers in Immunology, 12, 2021.

[3] G. Selvaggio et al., A quantitative systems pharmacology approach to support mRNA vaccine development and optimization, CPT: Pharmacometrics and Systems Pharmacology, 10.12: 1448, 2021.

[4] F. Liang et al., Efficient targeting and activation of antigen-presenting cells in vivo after modified mRNA vaccine administration in rhesus macaques, Molecular Therapy, 25.12: 2635-2647, 2017.

[5] The Wellcome Leap R3 project. https://wellcomeleap.org/r3/

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Multi-scale modelling of focal adhesions

Di Stefano Salvatore[*], Ramírez Torres Ariel[†], Bellino Luca[*], Fazio Vincenzo[#], Florio Giuseppe[*§], Puglisi Giuseppe[*]

[*]Dipartimento di Ingegneria Civile, Ambientale, del Territorio, Edile e di Chimica (DICATECh)
Politecnico di Bari
Bari, Italy
e-mail: {salvatore.distefano, luca.bellino, giuseppe.florio, giuseppe.puglisi}@poliba.it

[†]School of Mathematics and Statistics
University of Glasgow
Glasgow, United Kingdom
e-mail: ariel.ramireztorres@glasgow.ac.uk

[#]Laboratory for Bioinspired, Bionic, Nano, Meta Materials & Mechanics
Università degli Studi di Trento
Trento, Italy
e-mail: vincenzo.fazio@unitn.it

[§]INFN, Sezione di Bari
Bari, Italy

Abstract: We study the decohesion of cell-matrix systems, intending to highlight how the elastic properties of both cells and the extra-cellular matrix (ECM) modulate and drive the onset and progression of such a phenomenon. In this work, we particularise our research to focal adhesions (FAs), representing an integrin-mediated structure that oversees and guides the mutual interactions between cells and the ECM. More specifically, FAs determine a stable mechanical linkage between the adhesion plaque and the ECM through integrin receptors. The former is a multi-protein complex interacting with the inner environment of a cell by means of stress fibres, while the latter bind the ECM ligands and form molecular bonds with them. In our approach, we employ a two-scale asymptotic homogenisation technique to study the multi-scale nature of FAs and their intrinsic heterogeneity, associated with the presence of several types of proteins within the adhesion plaque, the non-uniform distribution of the integrin receptors and the complex internal structure of the ECM. The main result of our work is the definition of effective parameters encoding the intrinsic heterogeneous properties of both FAs and ECM and the obtaining of suitable homogenised field equations describing the effective behaviour of FAs undergoing rupture.

Keywords: focal adhesions; cell-matrix systems; asymptotic homogenisation; biological decohesion

1. Introduction

We specialize our study to focal adhesions (FAs), representing the basic sites by means of cells anchor to ECM and share chemo-mechanical signals with it [1-4]. We adhere to a purely mechanical model, even though other effects, such as temperature, should be considered, as is done in studying other biological situations [5-7]. We schematize the structure of a FA as a three-component system, comprising the adhesion plaque, integrin receptors and stress fibres [1,3,4] and we study how the elastic properties of the FAs and of the ECM influence the decohesion of the FA-ECM system [3,5]. In doing this, we develop a multi-scale approach, based on Asymptotic Homogenization [6,8].

2. The model

It is known that FA, ECM and integrins are typically non-heterogeneous [9] and such heterogeneity character is associated with length scales which are smaller than those

characterizing the whole FA-ECM complex. In other words, the system under investigation exhibits at least the co-existence of two main scales: the first one is typical of the heterogeneities of the components constituting the adhesion plaque, the ECM and the integrins, whereas the other one is representative of the system as a whole [9]. Such characteristic lengths, in addition, are well separated [6,8]. Accordingly, we employ a two-scale homogenization procedure to deduce the overall mechanical behaviour of the FA-ECM system in the case of decohesion. By referring to the mechanical picture outlined in [3] and by virtue of the scale separation condition discussed above, we re-interpret it in a two-scale fashion [8]. This leads us to formulate constitutive relations incorporating the information of the micro-structure and compute *homogenized* or *effective* elastic coefficients, encoding the elastic properties of FAs, ECM and integrins at the scale of the heterogeneities. Moreover, we infer a system of local field equations, describing the point-wise equilibrium of the considered physical system at the micro- and micro-scale, respectively.

3. Results

The effective elastic parameters are obtained as the solutions of suitable *cell equations*, in the jargon of Asymptotic Homogenization [8,9], by employing standard arguments of two-scale periodic analysis. We emphasize that the functional form of such cell equations depends on the considered mechanical model, describing the macro-scale mechanical interactions exchanged at the scale of the FA-ECM system and its decohesion, and on the way in which inhomogeneities are distributed at the microstructure.

References

[1] X. Cao, et al. A chemomechanical model of matrix and nuclear rigidity regulation of focal adhesion size. Biophysical Journal 109.9 (2015): 1807-1817.

[2] X. Cao, et al. Multiscale model predicts increasing focal adhesion size with decreasing stiffness in fibrous matrices. Proceedings of the National Academy of Sciences 114.23 (2017): E4549-E4555.

[3] S. Di Stefano, et al. On the role of elasticity in focal adhesion stability within the passive regime. Int. J. Non Linear Mech. 10.1016/j.ijnonlinmec.2022.104157 (2022)

[4] S. Di Stefano, E. Benvenuti, V. Coscia. On the role of friction and remodelling in cell-matrix interactions: A continuum mechanical model. Int. J. Non Linear Mech.142 (2022): 103966.

[5] L. Bellino, et al. On the competition between interface energy and temperature in phase transition phenomena, Application of Engineering Science, 2, 100009, (2020).

[6] A. Ramírez-Torres, et al. The role of malignant tissue on the thermal distribution of cancerous breast. Journal of Theoretical Biology 426 (2017): 152-161.

[7] V. Fazio, D. De Tommasi, N. M. Pugno, G. Puglisi, Spider Silks Mechanics: Predicting Humidity and Temperature Effects. JMPS, in print, (2022).

[8] N.S. Bakhvalov, G. Panasenko. Homogenisation: averaging processes in periodic media: mathematical problems in the mechanics of composite materials. Vol. 36. Springer Science & Business Media, 2012.

[9] Di Stefano, S., et al. Multiscale approach to decohesion in cell-matrix systems. AIMETA 2022 – Proceedings of the XXV conference of the Italian Association of Theoretical and Applied Mechanics. Accepted.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Using the SPH to Simulate the Process of Cell Proliferation

Barbosa Maria Inês[*], Belinha Jorge[†] Natal Jorge Renato[+] and Xavier Ana[°]

[*] Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI)
Universidade do Porto
Porto, Portugal
e-mail: up201405732@edu.fe.up.pt

[†] Department of Mechanical Engineering
Instituto Superior de Engenharia do Porto (ISEP)
Porto, Portugal
e-mail: job@isep.ipp.pt

[+] Department of Mechanical Engineering (DEMec)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: rnatal@fe.up.pt

[°] Institute for Research and Innovation in Health (I3S)
Universidade do Porto
Porto, Portugal
e-mail: anacarvalho@ibmc.up.pt

Abstract: A balance between cell proliferation and apoptosis is vital to maintain the homeostasis and a healthy human body. Cell proliferation is one of the main functions of cells and is characterized by its complexity. To study this process, besides the traditional experimental studies, computational models and simulations are used and considered a useful tool which helps in the progression of scientific research in this field. The present work proposes a new algorithm that simulates the process of cell proliferation using the Smoothed Particle Hydrodynamics method to solve it. In this work, two different analyses were made: one as a calibration and another to validate the algorithm. Besides that, individual cells and groups of cells were considered. In these analyses, the evolution of the volume growth, reproducibility and, for the groups of cells, the diameter, volume and form of the cluster were studied. In the end, it was possible to conclude that the algorithm was capable of mimicking both cell growth and division, led to exponential growth in the number of cells and generated coherent and similar results in all simulations.

Keywords: Numerical Simulation, Particle Method, Cell Proliferation, Cell Growth, Cell Division

1. Introduction

Cells have the capacity to proliferate. During the process of cell proliferation, cells grow and divide into two new genetically identical cells [1]. This process is quite complex and has yet to be fully understood. Besides the experimental studies, computational models have been proposed to support scientific research in this field and with them, predictions are made and new insights are followed [2]. To solve these models, numerical methods are usually used. The Smoothed Particle Hydrodynamics (SPH) method is one of the most well-known methods due to its simplicity and robustness in the execution of the kernel integration step [3]. In this work, a novel 3D non-linear iterative algorithm to simulate the process of cell proliferation is proposed. This algorithm is solved by the SPH and Navier-Stokes equations are used to derive and obtain the physical forces applied to the particles. The growth and division of individual cells and of a group of cells were tested and calibrated. Additionally, the diameter, volume and form of the group of cells were considered.

2. Methods

The SPH is a particle method and so, it uses particles without a pre-established connection to discretize the domain. Moreover, it constructs approximation functions to approximate the field function. In this case, these functions are applied to the Navier-Stokes equations. Concerning the proposed algorithm, initial input data is given and the particle discretization is created taking into account the three different types of particles defined in this work. Only one cell is considered in the beginning and the initial velocity, internal pressure and acceleration of the particles are obtained. Then, the cell starts to grow until it achieves the double of its initial volume and divides, creating a new particle. This process repeats for all cells and, in all iterations, kernel functions are constructed to update the particle positions.

3. Results

As previously mentioned, the growth of the initial cell and the total form, volume and diameter of the group of cells was analysed with the aim of calibrating and verifying the viability of the algorithm. For all these analyses, 20 iterative simulations were run and in all of them, 7 cell divisions occurred. When the growth of one cell is considered, a linear volume growth pattern was obtained and its division occurred after doubling its initial volume. The process of division generated exponential growth in the number of cells, as expected, since they followed the same process of growth and division throughout the iterations. For all simulations, the group of cells generated was similar. Although the position of the new cells was never the same due to the randomness of the process, the forms, diameters and volumes obtained were similar.

4. Conclusions

With the obtained results in the different simulations, it was possible to conclude that the algorithm is able to emulate the process of cell proliferation of one cell and a group of cells. The results were suitable and coherent with what was expected and with the data present in the literature. Besides that, the different simulations showed the reproducibility of the algorithm despite the randomness associated with it. Although it is still at an early stage, the algorithm seems to be a promising tool to simulate this kind of process. For future work, new improvements should be added to produce more complex and realistic simulations. For example, extracellular factors that influence the process of proliferation coud be introduced.

Acknowledgements

The authors acknowledge the funding provided by Ministério da Ciência, Tecnologia e Ensino Superior – Fundação para a Ciência e a Tecnologia (Portugal), under grants: SFRH/BD/146272/2019; and by LAETA, under project UIDB/50022/2020.

References

[1] Tortora GJ, Derrickson BH. Introduction to the human body. John Wiley & Sons, Incorporated; 2017.

[2] Banerjee S. Mathematical modeling: models, analysis and applications. Chapman and Hall/CRC; 2021.

[3] Liu GR, Liu MB. Smoothed particle hydrodynamics: a meshfree particle method. World scientific; 2003.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Poynting Effect in Weakly-Compressible Porous Cylinders in Torsion

Griffen Small*, Harold Berjamin† and Valentina Balbi‡

* School of Mathematical and Statistical Sciences
University of Galway
Galway, Ireland
e-mail: g.small1@universityofgalway.ie

† School of Mathematical and Statistical Sciences
University of Galway
Galway, Ireland
e-mail: harold.berjamin@universityofgalway.ie

‡ School of Mathematical and Statistical Sciences
University of Galway
Galway, Ireland
e-mail: vbalbi@universityofgalway.ie

Abstract: The aim of our work is the development of a mathematical model that can capture the Poynting effect in fluid immersed poro-elastic materials in torsion, which is lacking in the literature. The mechanical response of such a material, which consists of a incompressible, hyper-elastic solid skeleton whose pore space is saturated with an inviscid, incompressible fluid that is the same as the exterior fluid, can be described using mixture theory. Although both of its constituents are intrinsically incompressible, the poro-elastic material as a whole is compressible since it may gain or lose fluid through its pores, which necessitates the inclusion of compressibility effects in the finite hyper-elasticity analysis. Our model, a poro-elastic extension of the monophasic, incompressible models found in anterior studies, allows one to quantify the effect of the fluid and of the solid on the overall normal force and shows that the negative Poynting effect cannot be attributed to the poro-elastic nature of the material. In the case of a weakly-compressible Mooney-Rivlin skeleton, we present analytical expressions for the torque and normal force required to maintain the torsion deformation, and we compare the predictions of our model with those obtained from finite element simulations.

Keywords: Finite Deformations, Poynting Effect, Poro-Elasticity, Fluid-Saturated Media, Mixture Theory

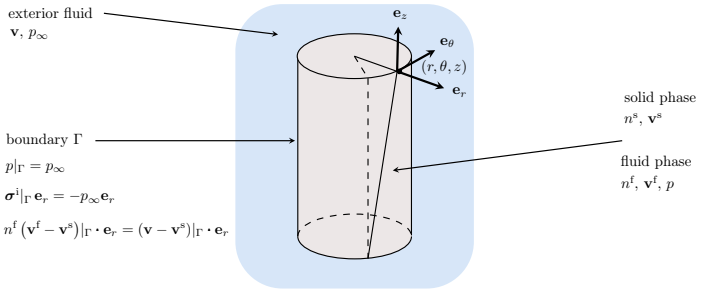


Figure 1: Deformed poro-elastic cylinder with appropriate boundary conditions, in cylindrical polar coordinates. Inside the cylinder there is a solid phase with volume fraction n^{s} and velocity $\mathbf{v}^{\mathrm{s}}$ and a fluid phase with volume fraction n^{f}, velocity $\mathbf{v}^{\mathrm{f}}$ and pressure p. The cylinder is immersed in a fluid with velocity $\mathbf{v}$ and pressure p_∞. Here, $\boldsymbol{\sigma}^{\mathrm{i}}$ is the sum of the fluid and solid stresses inside the cylinder.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Elasticity and force inclination effects for peeling phenomena

Binetti Claudia*, Bellino Luca*, Florio Giuseppe*, and Puglisi Giuseppe***

* Department of Civil, Environmental, Land, Building Engineering and Chemistry (DICATECh), Polytechnic University of Bari, via Orabona 4, 70125 Bari, Italy
** INFN, Sezione di Bari, I-70126, Italy

Abstract: We propose a peeling model consisting of a discrete lattice (the adhering layer) of elastically interacting units connected by breakable links to a rigid layer. Based on an energy minimization approach, we highlight the crucial role of governing parameters such as the relative elasticity of breakable and non breakable bonds as well as the angle and magnitude of the applied force. We believe that, at different lengthscales, the proposed model can be of interest both for describing different biological and natural processes and for the analysis of classical adhesion and decohesion effects in technological applications.

Keywords: Peeling, adhesion, non-convex energies, mechanical effects

The advent of single molecule experiments opened up the possibility of studying biological systems under different conditions of mechanical load, and it has been observed that the role of forces is crucial in many phenomena such as in the case of focal adhesions [1] (see Figure 1a). With the aim of understanding such complex systems under the action of mechanical forces, both continuum and discrete models have been introduced, successfully describing a large variety of biological problems, such as the cohesion-dechoesion asymmetry of gecko's pads [2], or even incorporating temperature effects to predict melting transitions in DNA [3].

In this work, following the approach in [2], recently extended to consider thermal effects in [4], we consider a prototypical model of a lattice of n elastically interacting massless points connected to a substrate by breakable elements, as shown in Figure 1b. Differently from [2] and [4], where only displacements orthogonal to the substrate have been considered, here we focus our attention on a fully two-dimensional system subjected to a variable force in inclination and magnitude. While this extension complicates the analytical treatment of the system, it is essential for the describing the fundamental effect of force inclination on the thermo-mechanical response of the decohesion phenomenon.

Specifically, the chain is made by n massless units connected each other by linear elastic springs each with associated energy $\phi_{el}(L_i) = 1/2\ k_{el}(L_i - \ell_0)^2$, with ℓ_0 the rest length, and linked to the substrate by elasto-fragile elements with energy $\phi_p(\theta_i, L_i) = 1/2\ k_p|\mathbf{S}_i(\theta_i, L_i)|^2$ (see Figure 1b). Here $\mathbf{S}_i(\theta_i, L_i)$ is the displacement vector of the $i-$th element, which behaves elastically up to a critical extension threshold $|\mathbf{S}_i(\theta_i, L_i)| = S_d$, and then suddenly breaks with the force jumping to zero. To describe this feature, we introduce an internal spin variable χ_i which assumes value $\chi_i = 1$ if the link is attached, and $\chi_i = 0$ if the link is broken, so that the total energy of the system reads

$$\phi\left(\{\theta_i\}, \{L_i\}\right) = \frac{1}{2} k_p \sum_{i=1}^{n} \left[\chi_i \left|\mathbf{S}_i(\theta_i, L_i)\right|^2 + (1 - \chi_i)\, S_d^2\right] + \frac{1}{2} k_{el} \sum_{i=1}^{n} (L_i - \ell_0)^2. \tag{1}$$

We analyze the thermo-mechanical response of the system when one end is anchored to the substrate and a force F with variable magnitude and inclination is applied to the other free

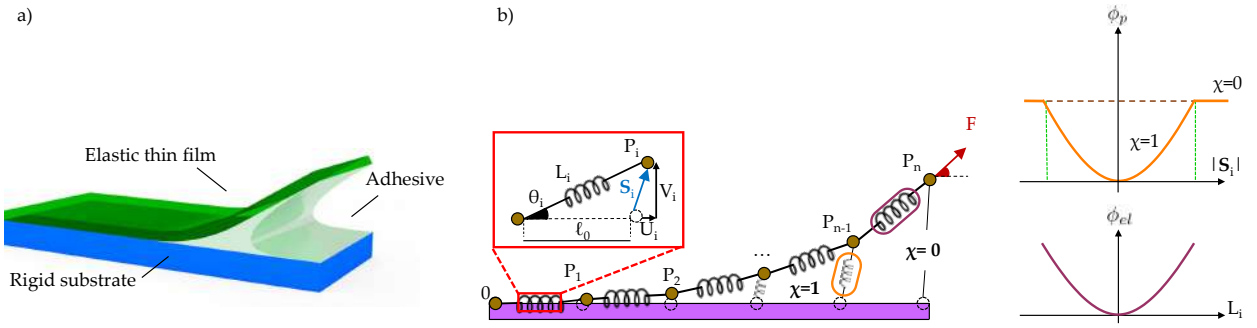


Figure 1: a) Schematic representation of an elastic thin film detaching from a rigid substrate. b) Mechanical model of n elastic springs (violet curve) connected to the substrate by breakable units (orange curve).

end. We study the effects of such parameters, including also the relative stiffness between the adhering and adhesive layers k_{el}/k_p and the role of temperature. Indeed, within a Statistical Mechanics framework, we define the canonical partition function of the system

$$\mathcal{Z} = \int_{\mathbb{R}^{2n}} e^{-\beta[\phi(\theta_i, L_i) - F\delta]} \mathrm{d}\theta_1 \dots \mathrm{d}\theta_n \mathrm{d}L_1 \dots \mathrm{d}L_n \tag{2}$$

where δ is the total displacement conjugate to the applied force F and $\beta = 1/(k_B T)$, with k_B the Boltzmann's constant and T the absolute temperature. Thus, it is possible to evaluate the temperature effects on the expectation values of physical observables, on the relation between the force experienced by the system and δ, the role of the mechanical parameters and, finally, analyze the temperature-dependent decohesion phenomenon.

Acknowledgements – LB, GF and GP are supported by 'Gruppo Nazionale per la Fisica Matematica' (GNFM) and by the Italian Ministry MIUR-PRIN project 2017KL4EF3. GF and GP are funded through the project PNRR, MISURA *M4C*21.4 - CAMPIONI NAZIONALI DI R&S National Centre for HPC, Big Data and Quantum Computing (CN00000013) - Spoke 5. GF is also supported by 'Istituto Nazionale di Fisica Nucleare' (INFN) through the project QUANTUM . LB is supported by "Progetto di Ricerca GNFM - INdAM", codice CUP-E53C22001930001.

References

[1] Cao, X., et al., Multiscale model predicts increasing focal adhesion size with decreasing stiffness in fibrous matrices, *Proceedings of the National Academy of Sciences*, 114(23), E4549-E4555, 2017.

[2] Puglisi, G. and Truskinovsky, L., Cohesion-decohesion asymmetry in geckos, *Physical Review* E, 87, 3, 032714, 2013.

[3] Florio, G., and Puglisi, G., A predictive model for the thermomechanical melting transition of double stranded DNA. *Acta Biomaterialia*, 157, 225-235, 2023.

[4] Bellino, L., et al., On the competition between interface energy and temperature in phase transition phenomena, *Applications in Engineering Science* 2, 100009, 2020.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A three-dimensional elasto-plastic biphasic model of multicellular aggregates

Di Stefano S.[1], **Giammarini A.**[2], **Giverso C.**[3], **Grillo A.**[4]

[1] Dipartimento di Ingegneria Civile, Ambientale, del Territorio, Edile e di Chimica (DICATECh)
Politecnico di Bari
Bari, Italy
e-mail: salvatore.distefano@poliba.it

[2,3,4]Dipartimento di Scienze Matematiche "G.L. Lagrange" (DISMA)
Politecnico di Torino
Turin, Italy
e-mail: alessandro.giammarini@polito.it
e-mail: chiara.giverso@polito.it
e-mail: alfio.grillo@polito.it

Abstract: We propose a mathematical model of multicellular aggregates and we specialise it to the case of uniaxial compression-release test. The multicellular aggregate is studied as a hydrated soft porous medium, in which we distinguish a solid phase, consisting of the overall contribution of the cytoskeleton, intracellular fluid and protein filaments, and a fluid phase that is constituted by the interstitial fluid. In particular, the behaviour of the solid phase is influenced by the phenomenon of remodelling, which is the process of reorganisation of the internal structure in response to the external compression. The fluid is assumed to be macroscopically inviscid and to be in Darcian regime. Finally, we formulate a contact problem to solve the exchange of mechanical interaction between the plates of the experimental apparatus and the multicellular aggregate. An evaluation of the influence of remodelling on fluid dynamics is carried out by considering both remodelling-independent permeability tensor and a dependent one. Our numerical simulations show an interplay between the fluid motion and the onset of remodelling, both for a direct and indirect coupling. In particular, the relation between the relevance of the coupling between the remodelling and the flow and elastic, hydraulic and remodelling parameters are investigated.

Keywords: Multicellular aggregates; Remodelling; Poro-plasticity; Contact problems.

This contribution is taken from [1] and concerns the modelling of multicellular aggregates, which can be thought as an ideal case of study for obtaining a better understanding of the underlying mechanics of tumors, for example [5]. Tumors interact remarkably with the environment surrounding them through biological processes of different nature and, in the early stages of their formation, the mechanical interactions take on a prominent role [2]. This motivates the study of simpler biological systems, like multicellular aggregates. A relevant framework for studying remodelling in multicellular aggregates is put forward in [6], in order to give a comprehensive mechanical description of the experiment.

1 Extended abstract content

A variety of modelling strategies for multicellular aggregates is present in the literature, depending on time and space scales. Since our purpose is the modelling of a compression-release experiments that lasts for minutes, we regard them as saturated biphasic media,

in which we distinguish a solid phase, which can undergo remodelling, and a fluid one (interstitial fluid), thereby fully reconsidering the model presented in [3]. Moreover, we request the mass and momentum balance of both phases and, for remodelling, we write an evolution law for the remodelling tensor based on a flow rule of Perzyna-type. The fluid phase is described in terms of Darcy's law, so that the motion of the fluid is known once the equation for the pressure field is solved, whilst the solid phase is isotropic, hyperelastic and subject to remodelling. In the summary of the model, $\boldsymbol{\sigma}^{(\mathrm{sc})}$ is the Cauchy stress tensor of the solid phase, $\boldsymbol{v}^{(\mathrm{s})}$ the velocity field of the solid phase, $\boldsymbol{a}_g$ the force density related to gravity, ρ the density of the mixture, $\varrho^{(\mathrm{f})}$ the density of the fluid, p the pressure field, $\boldsymbol{k}$ the permeability tensor, $\boldsymbol{b}_{\mathrm{e}}$ the remodelling tensor, γ_{p} concerns the triggering of the flow rule, $\boldsymbol{g}$ the metric tensor:

$$\operatorname{div} \boldsymbol{v}^{(\mathrm{s})} - \operatorname{div}[\boldsymbol{k}(\operatorname{grad} p - \varrho^{(\mathrm{f})} \boldsymbol{g} \boldsymbol{a}_g)] = 0, \qquad \text{in } \mathscr{B}(t), \tag{1}$$

$$\operatorname{div}(-p\boldsymbol{g}^{-1} + \boldsymbol{\sigma}^{(\mathrm{sc})}) + \rho \boldsymbol{a}_{\mathrm{g}} = \boldsymbol{0}, \qquad \text{in } \mathscr{B}(t), \tag{2}$$

$$\mathcal{L}\boldsymbol{b}_{\mathrm{e}} = -2\gamma_{\mathrm{p}} \boldsymbol{b}_{\mathrm{e}} \boldsymbol{g} \operatorname{dev} \boldsymbol{\sigma}^{(\mathrm{sc})}, \qquad \text{in } \mathscr{B}(t). \tag{3}$$

The plates of the experimental apparatus that compress the aggregate are modelled separately. We then prescribe appropriate boundary conditions for both the aggregate and the plates. In particular, a contact problem is formulated in the regions of the aggregate that are pressed by the plates [1, 3].

References

[1] Di Stefano, S., Giammarini, A., Giverso, C. et al. An elasto-plastic biphasic model of the compression of multicellular aggregates: the influence of fluid on stress and deformation. Z. Angew. Math. Phys. 73, 79 (2022).

[2] L. V. Garmanchuk, E. M. Perepelitsyna, M. V. Sydorenko, L. I. Ostapchenko. Formation of multicellular aggregates under different conditions of microenvironment. Cyt. Gen., 44, 19-22 (2010).

[3] C. Giverso, S. Di Stefano, A. Grillo, L. Preziosi, A three dimensional model of multicellular aggregate compression, Soft Matter, 15.48, 10005-10019 (2019).

[4] G. Forgacs, R. A. Foty, Y. Shafrir, M. S. Steinberg, Viscoelastic Properties of Living Embryonic Tissues: a Quantitative Study, Biop. Jour., 74, 2227-2234 (1998).

[5] Lisa D. Muiznieks, Fred W. Keeley. Molecular assembly and mechanical properties of the extracellular matrix: A fibrous protein perspective, Bioch. et Biophys. Acta (BBA), 7, 866-875 (2013).

[6] L. Preziosi, D. Ambrosi, C. Verdier. An elasto-visco-plastic model of cell aggregates, J. Theor. Biol., 262, 35-47 (2010).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A Hamilton principle-based model for diffusion-driven growth

Felix Klempt*, Meisam Soleimani* and Philipp Junker*

*Institute of Continuum Mechanics (IKM)
Fakultät für Maschinenbau, Leibniz Universität Hannover
Hannover, Deutschland
e-mail: junker@ikm.uni-hannover.de

Abstract: In an effort to enhance the durability of implants, especially oral implants, in-silico models proove to be a useful tool in supporting in-vitro and in-vivo experiments. To get accurate results from these in-silico models, the mathematical description needs to be physically and thermodynamically sound. By basing the mathematical description on the Hamilton principle, the presented model fulfills the first and second law of thermodynamics automatically. In literature, the second law of thermodynamics is often disregarded with biological growth models. In addition, the model combines the volumetric modeling approach with a density based one. The results show a good phenomenological agreement with what to be expected from growing biofilm.

Keywords: Biofilm growth, Multi-physics, FEM, Hamilton principle

1 Introduction

Inserted implants are always surrounded by biofilm forming microorganisms. These biofilms can become troublesome and can lead to implant failure. To prevent biofilm creation on implants, in-silico models are a cost effective way to provide data. Successful in-silico models need a sound physical foundation to be reliable. Prominent models in literature cannot show that the dissipation of energy in the system is positive disregarding the second law of thermodynamics. The model presented in this work is based on the Hamilton principle which grounds the model on the first and second law of thermodynamics. For further explanations on the extended Hamilton principle, the reader is refered to [1].

2 Mathematical model

The two main assumptions of the models are that growth and remodelling strongly impacts the energies of the biofilm and that the energy is transported by the nutrients. The growth state variable is introduced as $\phi(x) \in [0,1]$, where $\phi = 1$ is considered fully dense and $\phi = 0$ the absents of biofilm. Intermediate states are interpreted as partially dense biofilm. Equation 1 shows the weak form of the governing equation for the growth state variable. It consists of four terms: the change of density, a diffusion term, a term which links the growth parameter α to the density and a source term. The source term determines the direction of growth by the product of the gradient of the density and the normalized gradient of the nutrient concentration c: $\overline{\nabla c} = \frac{\nabla c}{\|\nabla c\|}$. It is scaled by the factor R_s and the Monod equation with the material parameters k_1 and k_2.

$$\delta\mathcal{G}_\phi = \int_\Omega (\dot{\phi} + \beta\,\nabla^2\phi + k_\alpha\alpha + R_s\frac{k_1 c}{k_2 + c}\,\nabla\phi\cdot\overline{\nabla c})\delta\phi\,dV = 0 \qquad \forall\delta\phi \tag{1}$$

The weak form of the governing equation for the nutrients is presented in equation 2. The first two terms are equivalent to equation 1, the third term is a sink term modelling the consumption of nutrients by the microorganisms. The consumption factor g is assumed to be constant.

$$\delta\mathcal{G}_c = \int_\Omega (\dot{c} + D\,\nabla^2 c + g\phi)\,\delta c\,dV = 0 \qquad \forall \delta c \tag{2}$$

Lastly, the strain energy function in equation 3 completes the model. The first term enforces incompressibility of the biofilm with the Lagrange parameter p, which is interpreted as hydrostatic stress. The second term describes the energy of the mechanical body of the biofilm.

$$\Psi_e(\mathbf{F}, \mathbf{F}_g^{-1}) = \mathrm{p}\,(\det(\mathbf{F}_e) - 1) + \phi^2 \frac{\mu}{2}\,\mathrm{tr}(\tilde{\mathbf{C}}_e - 3) \tag{3}$$

Figure 1 shows the end of a simulation where the biofilm started as a small ball in the center of the discretized cube and the nutrients are located in one corner. It can be observed that the biofilm growth in the direction of the nutrients, as intended by equation 1.

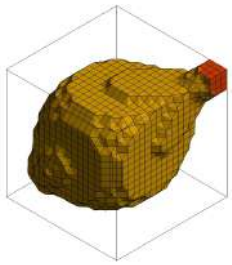


Figure 1: Capped isosurface of the growth state variable ϕ with a value larger than $0,878$. The growth towards the corner with the nutrients is easily identifiable.

3 Conclusion

With the described approach, it was possible to combine volumetric and density based growth equation into one coherent model. Additionally, this model is based upon the first and second law of thermodynamics. It shows good qualitative agreements with what to be expected from a growing biofilm. In the future, the material parameters have to be selected for specific bacteria in order to compare the simulation result to in-vitro experiments.

4 Acknowledgements

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – SFB/TRR-298-SIIRI – Project-ID 426335750

References

[1] Junker P, Balzani D. An extended hamilton principle as unifying theory for coupled problems and dissipative microstructure evolution. Continuum Mechanics and Thermodynamics 2021;33:1931-56

[2] Rodriguez EK, Hoger A, McCulloch AD. Stress-dependent finite growth in soft elastic tissues. Journal of biomechanics 1994;27:455-67

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Instability Analysis of Functionally-Graded Thin Auxetic Materials[¶]

Sairam Pamulaparthi Venkata[*,†], **Michel Destrade**[†,§], **Valentina Balbi**[†], **Dino Accoto**[‡], **and Giuseppe Zurlo**[†]

[†] University of Galway
Galway, Ireland
s.pamulaparthivenkata1@universityofgalway.ie, vbalbi@universityofgalway.ie,
giuseppe.zurlo@universityofgalway.ie,

[§] Zhejiang University
Hangzhou, People's Republic of China
michel.destrade@universityofgalway.ie

[‡] KU Leuven
Leuven, Belgium
dino.accoto@kuleuven.be

Abstract: Materials with negative Poisson's ratio belong to the so-called auxetic material class: they display exotic properties such as contraction/expansion in all directions under uniaxial compression/tension. They are found in a wide range of applications in robotics, and in structural, aerospace, and biomedical engineering. Hence, understanding their stability/instability response is essential for their design. We illustrate how spatial variations in the material properties of an auxetic membrane affect the type of instability experienced (snap-through, wrinkling and necking) under various loading conditions. To describe wrinkling, we employ a relaxed strain energy function, and we show that material inhomogeneities can be tailored to specify the locations and patterns of wrinkling in auxetic membranes. Using membrane theory, we also derive universal insights for inflated isotropic auxetic membranes, and we corroborate the theoretical insights with Finite Element (COMSOL) simulations. These results will help the deployment of functionally-graded auxetic membranes, for applications where inflated or laterally pulled membranes may be morphed and corrugated on demand.

Keywords: Auxetic membranes, Functionally-graded materials, Relaxed strain energy, Wrinkling, Necking

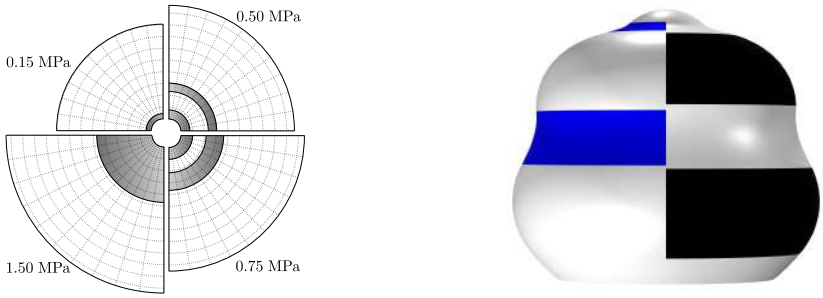


Figure 1: (a) Wrinkling profiles (grey) in a quadrant of a circular membrane with increase in the traction load. **(b)** Necking (blue) vs Wrinkling (black) in inflated circular membrane.

[¶] This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 956401.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A hybrid model of Tumors-on-chip: a numerical study

Campanile Elio[*,†], **Bretti Gabriella**[1], **Natalini Roberto**[1], **Menci Marta**[2]

[*] Fondazione The Microsoft Research - University of Trento Centre for Computational and Systems Biology (COSBI), Rovereto, Italy
e-mail: campanile@cosbi.eu

[†] Department of Mathematics, University of Trento, Trento, Italy
e-mail: elio.campanile@unitn.it

[1] Istituto per le Applicazioni del Calcolo "M.Picone", Rome, Italy

[2] Università Campus Bio-Medico di Roma, Rome, Italy

Abstract: In this talk a hybrid model for collective cell migrations will be presented. The approach is numerical, based on finite difference simulations and sensitivity analysis of the main model's parameters.

Keywords: Mathematical biology, Cell migration, Microfluidic chip, Finite difference numerical scheme.

1 Overview of the talk

During the last decades, mathematical modeling has become a powerful asset to explore biological phenomena and to detect obvious but also hidden mechanisms that might not have been known previously based solely on experiment observations. Among the many applications of mathematical modeling in biology, it is of great importance the study of cell migration, which consists of the directed movement of a single cell or a group of cells in response to chemical and/or mechanical signals.
In this talk, we explore a hybrid mathematical model based on an Organ-on-chip experiment using a discrete in continuous approach to mimic immune cells(ICs) migration towards tumor cells(TCs).
Organ-on-Chips (OOC) are recently-developed microfluidic chips that simulates the activities, mechanics and physiological response of an entire organ or an organ system. This allows microfluidic chips to reproduce in vivo systems on an in vitro system.
The work presented here refers to the experiments of Vacchelli et al.([4], [3]), where time-lapse imaging of microfluidic cocultures was performed to visualize motility patterns and interactions between chemotherapy-treated cancer cells and immune cells carrying different genetic variants of the FPR1 gene.
In [1], a fully macroscopic mathematical partial differential equation (PDE) model was considered, both for the chemical gradient, which is seen as an average field, and for the density of ICs. Our approach is hybrid: discrete for the particles and continuous for the molecular level involving the concentration of the chemical signal released by TCs in the environment. The advantage of a multiscale approach is twofold: on the one hand, we can turn our gaze within the chip and look at immune cells like single entities whose movement is ruled by specific forces. On the other hand, the presence of cancer cells involves the release of chemical substances that must be interpreted as an average on the space, hence naturally involving

a macroscopic scale of description. The model couples a reaction-diffusion partial differential equation describing the evolution of the average substances released by the TCs in the tumor micro-environment with a particle model. In particular, the dynamics of each IC are modelled by means of ordinary differential equations (ODE) in such a way that every cell can be followed individually. Since the motion of ICs is driven by chemotaxis, the migratory activity is regulated by a chemotactic term which allows them to sense the gradient of the chemicals in the tumor neighbourhood and by mechanical interactions occurring among cells.
The model improves previous works of the literature considering an additional alignment term influencing the ICs dynamics. In particular, we assume that the force acting on every particle is a weighted average of the differences of its velocity with those of the neighbouring particles. Moreover, the model accounts for a stochasticity component related to the motion of TCs cells, which are not fixed but their positions slightly change over time according to a Brownian motion.
Considering the variety of the model, multiple rigorous numerical schemes have been adapted or developed in order to simulate the coupled model. For the dynamics of the ICs, expressed by ODE, an IMEX(implicit-explicit) approach has been developed to combine an implicit scheme for the stiff components with an explicit scheme for the nonstiff components. For the chemical signal, expressed by PDE, a central difference scheme has been applied in space, while a $\theta-$method has been adopted in time.
A sensitivity analysis of the main model's parameters will be presented, especially for the ones that cannot be measured on experimental basis. Several numerical simulations will be shown in order to investigate the effect of the different interactions on the overall dynamics. The obtained numerical results show a good level of agreement with the observed phenomena.

References

[1] Braun EC, Bretti G, Natalini R. Mass-Preserving Approximation of a Chemotaxis Multi-Domain Transmission Model for Microfluidic Chips. Mathematics 2021;9(6):688.

[2] Bretti G, De Ninno A, Natalini R, Peri D, Roselli N. Estimation Algorithm for a Hybrid PDE–ODE Model Inspired by Immunocompetent Cancer-on-Chip Experiment. Axioms 2021;10(4):243.

[3] Businaro L, De Ninno A, Schiavoni G, et al. Cross talk between cancer and immune cells. Lab on chip 2013; 13(2):229-39.

[4] Vacchelli E et al. Chemotherapy-induced antitumor immunity requires formyl peptide receptor 1. Science 2015; 350(6263):972-8.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A kinetic study of contact guidance and steric hindrance interplay during cell migration

Conte Martina* **and Loy Nadia**†

* Department of Mathematical Sciences "G. L. Lagrange"
Politecnico di Torino
Torino, Italy
e-mail: martina.conte@polito.it

† Department of Mathematical Sciences "G. L. Lagrange"
Politecnico di Torino
Torino, Italy
e-mail: nadia.loy@polito.it

Abstract: We propose a non-local model for studying the twofold way effect of the extracellular matrix on polarization and speed of motion of the cells. Precisely, we model contact guidance and steric hindrance depending on this single external cue. Starting from a microscopic description of the stochastic cell re-orientation mechanism, we formally derive the corresponding kinetic equations for cell collective motion and its possible macroscopic limits in the appropriate regime. We test our model in several scenarios, comparing its outcomes with experimental results and showing its potential applicability.

Keywords: Non-local model, Kinetic transport equations, Steric hindrance, Contact guidance

1 Introduction

In several physiological and pathological situations, cells perform directed motion in response to external stimuli by sensing the environment with their membrane protrusions. Precisely, several biochemical and biophysical cues may give rise to direct migration towards specific targets. This defines a multi-cue environment in which cells have to sort and combine different, and potentially competitive, stimuli. In this work, we focus on the influence of the extracellular matrix (ECM), developing a non-local model for cell migration where a single cue has a twofold way effect on movement. Precisely, we analyze how this single cue can affect the polarization and speed of motion of the cells, looking at the interplay between contact guidance and steric hindrance.

2 Extended abstract content

Starting from the work in [1, 2], we aim at describing the effects of two different processes, both depending on the ECM, on the speed and the polarization of the cell. We consider a statistical description of ECM, given in terms of its macroscopic density and statistical distribution of the fiber direction, both non-locally evaluated. Precisely, the former is assumed to affect cell speed, the latter modifies cell direction, while the non-locality allows us to take into account the extension of cell protrusions, which are a great determinant of cell behavior in the presence of strongly heterogeneous or anisotropic environments [3].

We firstly state a microscopic discrete in time stochastic process to describe the underlying cell re-orientation mechanisms. From it, taking advantage of classical tools of kinetic theory, we formally derive the corresponding kinetic model that implements exactly the microscopic dynamics and we obtain the related macroscopic equation in the appropriate regime on the basis of the observed experimental parameters. Then, we numerically test our model in several scenarios, using it to obtain both quantitative and qualitative results. Precisely, we investigate the minimal microscopic mechanisms that are necessary to reproduce specific cell dynamics by comparing the outcomes of our model with experimental results related to breast cancer cell migration. Moreover, we use it to mimic the invasion of breast cancer cells from an aggregate into the collagen, according to the experiments presented in [4], and comparing the results of the microscopic, kinetic, and macroscopic models. An example of the results obtained in this case is shown in Figure 1. Finally, we show the model potential

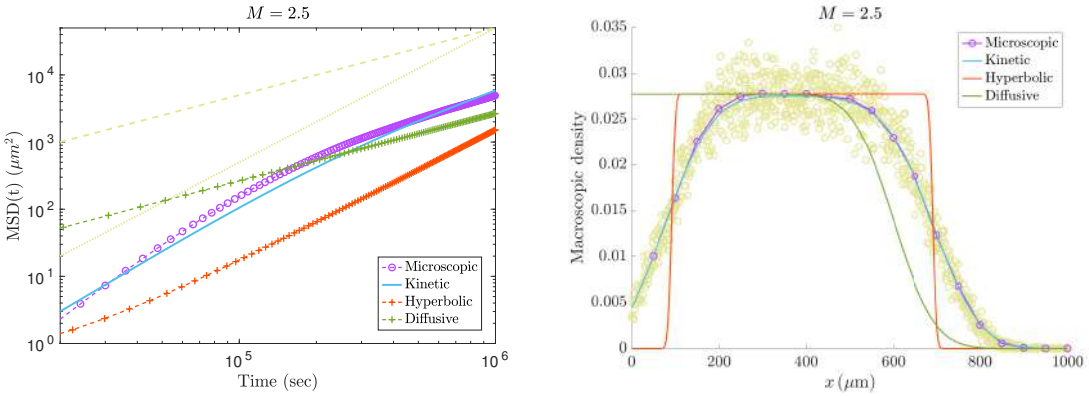


Figure 1: Mean squared displacement (MSD) comparison (left plot) and profile solutions (right plot)

applicability in the case of a heterogeneous environment with an interface dividing regions with different collagen densities and/or fiber alignment.

References

[1] Loy N, Preziosi L. Kinetic models with non-local sensing determining cell polarization and speed according to independent cues, J Math Biol, 2020; 80(1):373–421.

[2] Loy N, Preziosi L. Modelling physical limits of migration by a kinetic model with non-local sensing, J Math Biol, 2020; 80(6):1759–801.

[3] Han W, Chen S, Yuan W, Fan Q, Tian J, Wang X, Chen L, Zhang X, Wei W, Liu R, Qu J. Oriented collagen fibers direct tumor cell intravasation. PNAS, 2016;113(40):11208–13.

[4] Tien J, Ghani U, Dance YW, Seibel AJ, Karakan M, Ekinci KL, Nelson CM. Matrix pore size governs escape of human breast cancer cells from a microtumor to an empty cavity. Iscience, 2020;23(11):101673.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Privacy and Cooperation in Multi-Agent Distributed Systems

Fioravanti Camilla* **and Oliva Gabriele***

* Department of Engineering
University Campus Bio-Medico of Rome
Via Alvaro del Portillo, 21 - 00128 Roma, Italy
Email c.fioravanti@unicampus.it, g.oliva@unicampus.it

Abstract: Distributed agreement dynamics have always played a predominant role in the context of artificial multi-agent systems, as they allow an overall result to be achieved on the basis of partial exchanges. However, when considering modern application contexts in which agents also have competing interests, the dynamics of cooperation involving the constant sharing of information, typical of consensus-type algorithms, clash with each agent's need to preserve the privacy of its initial conditions. In addition to this, another emerging problem concerns possible break-in attempts by third parties and the destructive influence these have on the collective dynamics of the agents. Consequently, the implementation of algorithms that can effectively achieve the agreement while preserving privacy and protecting the network from external incursions becomes a matter of paramount importance. The contribution aims to provide a control theoretical analysis of the matter at hand, including a simulation campaign to illustrate the effectiveness of the proposed techniques.

Keywords: Consensus Algorithms, Distributed Algorithms, Multi-Agent Systems, Privacy Preservation

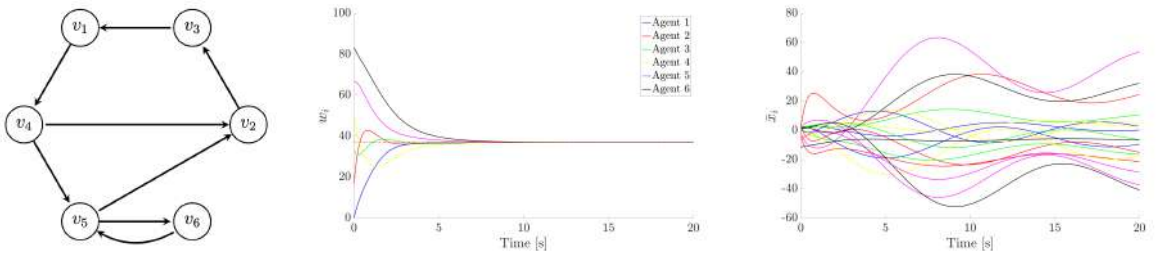
1 Introduction

In the context of distributed multi-agent systems, one of the main requirements is the achievement of a global agreement, based on the knowledge that each agent has of its own state and that of its neighbors. Distributed agreement algorithms such as consensus [1] represent a powerful framework to compose different pieces of information, with important applications ranging from noise reduction to distributed estimation and mobile robot coordination. Though effective, such methods suffer a lack of guarantees in terms of *privacy preservation*, in that agents exchange their states, thus sharing potentially sensitive information with their neighbors. This aspect becomes especially relevant when the agents have concurrent or competing interests, as in the context of Industrial Internet of Things (IIoT) networks, where the information handled is particularly sensitive. Placing ourselves in the case where agents exchange sensitive data on the network, another issue we must take into account concerns the possibility of eavesdropping or external intrusion by third parties, which can potentially compromise if not destroy the agreement.

2 Proposed Approach

Let us consider a network of n agents, interconnected by a graph $G = \{V, E\}$. Suppose each agent i holds an initial condition $w_i(0) = w_{i0}$ and is designed to interact with its neighbors according to the protocol

$$\dot{w}_i(t) = \sum_{j \in \mathcal{N}_i^{\text{in}}} (w_j(t) - w_i(t)) \,. \tag{1}$$



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

Figure 1: (a) Graph topology. (b) Temporal evolution of the hidden states $w_i(t)$. (c) Temporal evolution of the augmented states $\bar{\boldsymbol{x}}_i(t)$.

It is well known [1] that, if G is directed and strongly connected, then the agents asymptotically reach an agreement such that $\lim_{t\to\infty} \boldsymbol{w}(t) = \mathbf{1}_n \boldsymbol{\xi}^T \boldsymbol{w}(0)$, whereby all the agents reach consensus to a weighted average of their initial conditions, where the weights correspond to the entries of $\boldsymbol{\xi}$, the left eigenvector of the Laplacian matrix of G. Starting from this interaction rule, we developed a consensus strategy [2] that relies upon state augmentation and coordinate shifts and allows legitimate agents to securely interact with each other while avoiding disclosing their states $w_i(t)$ and the consensus value to malicious listeners. Specifically, with the aim to mask the consensus process, each agent maintains and exchanges (according to an interaction rule equivalent to the one in Eq.(1)) an augmented state $\overline{\boldsymbol{x}}_i(t) \in \mathbb{R}^m$ obtained by the use of a transformation matrix $T_i \in \mathbb{R}^{m\times m}$ that allows the state's coordinates to shift and the change of its dimensions

$$T_i \overline{\boldsymbol{x}}_i(t) = \begin{matrix} \boldsymbol{q}_i^T \overline{\boldsymbol{x}}_i(t) \\ Q_i \overline{\boldsymbol{x}}_i(t) \end{matrix} = \begin{matrix} w_i(t) \\ * \end{matrix} . \tag{2}$$

Figure 1 reports the hidden and visible evolution of the agents' state variables, obtained by simulating the application of our algorithm. Notably, as shown in Figure 1b, the agents successfully compute the intended weighted average while hiding their states $w_i(t)$. We complement our framework by providing an additional layer of protection against honest but curious legitimate agents, preventing them from gaining insights into the initial condition of their peers. To this end, we have developed several strategies, based on the addition of disturbance signals [2] or chaotic components [3] to each agent's hidden state.

References

[1] R. Olfati-Saber and R. M. Murray, "Consensus problems in networks of agents with switching topology and time-delays," *IEEE Transactions on Automatic Control*, vol. 49, no. 9, pp. 1520–1533, 2004.

[2] C. Fioravanti, L. Faramondi, G. Oliva, and C. N. Hadjicostis, "A Geometrical Approach for Consensus Security," *Systems & Control Letters*, Submitted.

[3] C. Fioravanti, G. Oliva, S. Panzieri, and C. N. Hadjicostis, "Private consensus using chaotic oscillator-based encryption," in *2022 IEEE Mediterranean Conference on Control and Automation (MED)*, 2022, pp. 927–932.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Robust control of interacting multi-agent systems under uncertainty

Giacomo Albi*, Michael Herty† and Chiara Segala+

* Department of Computer Science
University of Verona
Verona, Italy
e-mail: giacomo.albi@univr.it

† IGPM
RWTH Aachen University
Aachen, Germany
e-mail: herty@igpm.rwth-aachen.de

† IGPM
RWTH Aachen University
Aachen, Germany
e-mail: segala@igpm.rwth-aachen.de

Abstract: We consider control strategies for large–scale interacting agent systems under uncertainty. The particular focus is on the design of robust controls that allow to bound the variance of the controlled system over time. To this end we consider $\mathcal{H}_\infty$ control strategies on the agent and mean field description of the system. We show a bound on the $\mathcal{H}_\infty$ norm for a stabilizing controller independent on the number of agents. Furthermore, we compare the new control with existing approaches to treat uncertainty by generalized polynomial chaos expansion. Numerical results are presented for one-dimensional and two–dimensional agent systems.

Keywords: Collective agent-based dynamics, mean-field equations, uncertainty quantification, stochastic Galerkin, $\mathcal{H}_\infty$ control

1 Extended abstract content

We consider the mathematical modelling and control of phenomena of collective dynamics under uncertainties. These phenomena have been studied in several fields such as socio-economy, biology, and robotics [1, 5]. Those particles interact according to a possibly non-linear model, encoding various social rules as attraction, repulsion, and alignment. Understanding the impact of control inputs in such complex systems is of great relevance for applications [3, 7]. Further, the introduction of uncertainty in the mathematical modelling of real-world phenomena seems to be unavoidable, since often at most statistical information of the modelling parameters is available [2].

Here, we are concerned with the robustness of controls influencing the evolution of a collective motion of an interacting agent system under external uncertainty. More precisely, we consider the control of high-dimensional dynamics accounting N agents with state $v_i(t,\theta) \in \mathbb{R}^d$, $i =$

$1, \dots, N$, evolving according to

$$\frac{d}{dt} v_i(t,\theta) = \sum_{j=1}^{N} a_{ij}(v_j(t,\theta) - v_i(t,\theta)) + u_i(t,\theta) + \sum_{k=1}^{Z} \theta_k \,, \qquad v_i(0) = v_i^0, \tag{1}$$

where $A = [a_{ij}] \in \mathbb{R}^{N\times N}$ defines the nature of pairwise interaction among agents, and $\theta = (\theta_1, \dots, \theta_Z)^\top \in \mathbb{R}^{Z\times d}$ is a random input vector with a given probability density distribution on Z as $\rho \equiv \rho_1 \otimes \dots \otimes \rho_Z$. The control signal $u_i(t,\theta) \in \mathbb{R}^d$ is designed to stabilize the state toward a target state $\bar{v} \in \mathbb{R}^{N\times d}$, and its action is influenced by the random parameter θ. Of particular interest will be controls designed via minimization of linear quadratic (parametric) regulator functional such as

$$\min_{u(\cdot\,\theta)} J(u; v^0) := \int_0^{+\infty} \exp(-r\tau) \left[v^\top Q v + \nu u^\top R u \right] \, d\tau, \tag{2}$$

with Q positive semi-definite matrix of order N, R positive definite matrix of order N and r is a discount factor. In this case, the linear quadratic dynamics allow for an optimal control u^* stabilising the desired state $v_d = 0$, expressed in feedback form, and obtained by solving the associated matrix Riccati equations.

In order to assess the performances of controls, and quantify their robustness we propose estimates using the concept of $\mathcal{H}_\infty$ control [6]. Here we will study an approach based on the derivation of sufficient conditions in terms of linear matrix inequalities (LMIs) for the $\mathcal{H}_\infty$ control problem. In this way, consensus robustness will be ensured for a general feedback formulation of the control action. Additionally, we consider the large–agent limit and show that the robustness is guaranteed independently of the number of agents.

Furthermore, we will discuss the numerical realization of system (1) employing uncertainty quantification techniques [4]. The methods, here developed, make use of the stochastic Galerkin (SG) for the microscopic dynamics while in the mean-field case we combine SG in the random space with a Monte Carlo method in the physical variables.

References

[1] G. Albi, N. Bellomo, L. Fermo, S.-Y. Ha, J. Kim, L. Pareschi, D. Poyato, and J. Soler. Vehicular traffic, crowds, and swarms: from kinetic theory and multiscale methods to applications and research perspectives. *Math. Models Methods Appl. Sci.*, 29(10):1901–2005, 2019.

[2] J. A. Carrillo, L. Pareschi, and M. Zanella. Particle based gPC methods for mean-field models of swarming with uncertainty. *Communications in Computational Physics*, 25(2):508–531, 2018.

[3] E. Cristiani, B. Piccoli, and A. Tosin. *Multiscale modeling of pedestrian dynamics*, volume 12 of *MS&A. Model. Simul. Appl.* Springer, Cham, 2014.

[4] G. Dimarco, L. Pareschi, and M. Zanella. Uncertainty quantification for kinetic models in socio–economic and life sciences. In *Uncertainty quantification for hyperbolic and kinetic equations*, pages 151–191. Springer, 2017.

[5] M. Herty and L. Pareschi. Fokker-Planck asymptotics for traffic flow models. *Kinet. Relat. Models*, 3(1):165–179, 2010.

[6] Y. Luo and W. Zhu. Event-triggered h-infinity finite-time consensus control for nonlinear second-order multi-agent systems with disturbances. *Advances in Difference Equations*, 2021(1):1–19, 2021.

[7] A. Tosin and M. Zanella. Kinetic-controlled hydrodynamics for traffic models with driver-assist vehicles. *Multiscale Model. Simul.*, 17(2):716–749, 2019.

Abstract

The proliferation of fake news, which aims to manipulate individuals' perceptions of facts, has become a pressing concern in many democratic societies. To understand this phenomenon, we adopt a compartmental approach inspired by epidemiology and present two distinct kinetic models. Our focus is on how factors such as competence and learning influence the dissemination of misinformation, and how they contribute to the polarization of opinions within closed online communities. Both models allow us to study the spread of fake news through the lens of Fokker-Planck type surrogate models, which are then solved using a structure-preserving numerical scheme.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Computational modeling of pharmacokinetics and pharmacodynamics during in stent restenosis following drug-eluting stent implantation

Kiran Manjunatha*, Anna Ranno†, Marek Behr†, Felix Vogt†† and Stefanie Reese*

* Institute of Applied Mechanics (IFAM)
RWTH Aachen University
Aachen, Germany
e-mail: manjunatha@ifam.rwth-aachen.de

† Chair for Computational Analysis of Technical Systems (CATS)
RWTH Aachen University
Aachen, Germany
e-mail: ranno@cats.rwth-aachen.de

† Department of Cardiology, Pulmonology, Intensive Care and Vascular Medicine (CARD)
RWTH Aachen University
Aachen, Germany
e-mail: fvogt@ukaachen.de

Abstract: Percutaneous coronary intervention (PCI) is a minimally invasive procedure wherein the plaque built up within the coronary arteries, as part of an inflammatory pathosis termed atherosclerosis, is compressed against the coronary arterial walls using balloon angioplasty, and subsequently, a supporting scaffold called a stent is placed to restore normal blood flow within the coronary artery. Endothelial denudation and overstretch injuries caused during the PCI procedure kick start various signaling cascades within the arterial wall resulting in uncontrolled tissue growth and formation of obstructions to the blood flow. The condition is termed in-stent restenosis and the mechanism associated is called neointimal hyperplasia. Although the advent of drug-eluting stents (DES) was expected to eradicate the occurrence of restenosis, the probability of its occurrence remains statistically significant. This is suspected mainly due to the growth-inhibitory mechanisms acting indiscriminately on the smooth muscle cells as well as the endothelial cells, delaying the healing of the endothelium. The current work is thus aimed at extending the modeling framework developed by the authors to include the spatiotemporal effects of endothelium recovery in the arterial wall and to thus capture the pharmacokinetics and pharmacodynamics of drug elution from the stent surfaces. The extended high-fidelity model could then serve as an in silico tool for interventional cardiologists to tune DES implantation parameters including stent overtstretch, drug load on the DES as well as the post operative therapeutic regimens.

Keywords: in-stent restenosis, drug-eluting stents, smooth muscle cells, endothelial cells, pharmacokinetics, pharmacodynamics

Domain Size Impact on the Simulation of Intracranial Aneurysm Haemodynamics

P. Jeken Rico*, A. Goetz, A. Larcher, E. Hachem

* pablo.jeken_rico@minesparis.psl.eu

PSL Mines Paris, CFL Research Group at CEMEF, Sophia Antipolis, 06904, France

ABSTRACT

Introduction. Haemodynamics simulations of the human arterial system are seen as a potential tool to answer open questions about the initiation and progression of vascular diseases. Diseases, such as Intracranial Aneurysms (IA), pose a special challenge due to their delicate location and the lack of measurements to enrich simulations [1]. One of the necessary components to obtain physiologically accurate flow profiles is adequately simulating the peripheral flow surrounding the region of interest. To further develop this topic, this study assesses the influence of different 3D domain extensions on IA haemodynamics.

Methods. The three geometries of the Circle of Willis are investigated, each harbouring at least one IAs. The segmented geometries are varied progressively by reducing their spatial extension, yielding three levels of depth. In each case, the incompressible Navier-Stokes equations are solved numerically using a variational multiscale type finite element discretization [2]. The naturally occurring shear-thinning rheology of blood is mimicked through the Carreau-Yasuda model. Outlet boundary conditions are derived from the Principle of Minimum Work and transformed into pressure conditions. The results are compared by inspecting the flow structures and common risk indicators, such as the Wall Shear Stress (WSS) and the oscillatory shear index.

Results. Results show that locally constrained arterial trees can in some cases lead to considerable differences in flow patterns, even in qualitative terms. The alterations of the flow are consistent with the changes of fluxes at the aneurysm's bifurcation and are therefore highly case-dependent. The WSS accordingly changes in magnitude and location following the change of the primary variables. Oscillatory shearing is mostly present in low WSS regions of the dome and is traced back to the chaotic intralobular flow patterns.

Discussion. Presented results show that the choice of domain extension can be of importance in some cases and thus should be considered. IAs located at either of the posterior communicating arteries have to be treated carefully since no general boundary condition model for this vessel type has been established by the research community. The work confirms that simulation parameters, such as the size of the domain, can cause considerable inter-patient variability [3] and should be treated following a unified strategy.

REFERENCES

[1] H. Meng et. al. High WSS or Low WSS? Complex interactions of hemodynamics with intracranial aneurysm initiation, growth, and rupture: Toward a unifying hypothesis. *American Journal of Neu-*

roradiology, 2014.

[2] E. Hachem et. al. Stabilized finite element method for incompressible flows with high Reynolds number. *Journal of Computational Physics*, 2010.

[3] P. Paritala et. al. Reproducibility of the computational fluid dynamic analysis of a cerebral aneurysm monitored over a decade. *Nature Scientific Reports*, 2023.

The potential benefits of modelling arterial compliance for intracranial aneurysm risk assessment

A. Goetz[†,*], **P. Jeken-Rico**[†], **R. Nemer**[†], **A. Larcher**[†], **E. Hachem**[†]

[*] aurele.goetz@mines-paristech.fr

[†] PSL Mines Paris, CFL Research Group at CEMEF, Sophia Antipolis, 06904, France
ERC-2021-COG CURE 101045042

ABSTRACT

Introduction. Intracranial Aneurysms (IAs) are pathological dilations of arteries that bear the risk of rupture and subsequent subarachnoid haemorrhage. When diagnosed, they raise the question of a potential clinical intervention, which also entails a non-negligible threat. As a result, risk-evaluation tools are required to assess IAs' stability and aid physicians in their decision-making process. For this purpose, methods based on Computational Fluid Dynamics (CFD) have been developed to provide patient-specific indicators. However, CFD simulations of haemodynamics rely on multiple hypotheses and sources of error. Among them, the rigid wall assumption is mostly employed. Arterial tissue is commonly regarded as fully rigid and only a few research studies consider elastic or hyperelastic modelling with fluid-structure coupling. The scarce literature covering Fluid-Structure Interaction (FSI) in IAs mostly investigates complex patient-specific geometries [1]. This, along with different modelling assumptions, undermines comparisons between studies, thereby limiting the progress in the field. Idealized geometries of IAs have been investigated through CFD simulations [2], showing the impact of various geometrical parameters on the resulting haemodynamics. However, simple test cases are still missing for studying the FSI-related phenomena in a more controlled manner.

Methods. We introduce an idealized sidewall aneurysm geometry for simulating the interaction between a solid membrane and the impinging blood flow arising from a curved artery. The simplicity of the proposed case offers a perfect environment to assess the system's sensitivity with respect to a large span of physical parameters. Of particular interest are the vessel material properties and wall thickness, which vary substantially among previously published studies. We introduce our FSI simulation framework, which is based on a finite-element strongly-coupled partitioned approach that relies on an Arbitrary Lagrangian-Eulerian (ALE) formulation for the fluid and an updated Lagrangian solid solver further described in [3]. The incompressible Navier-Stokes equations are solved using a non-Newtonian blood rheology model and typical haemodynamic metrics such as the Wall Shear Stress (WSS) and the Oscillatory Shear Index (OSI) are computed in the different investigated configurations.

Results. Focus is drawn on the impact of physical and geometrical parameters of the simplified model on the measured WSS and OSI, metrics classically associated with aneurysm growth and rupture. By comparing the FSI simulations with a CFD reference case, we evaluate the limits of the rigid wall assumption. FSI modelling proves relevant when the arterial compliance is high enough to trigger a strong interaction with the fluid flow, thus altering its circulation. The presented results give a first insight towards the identification of aneurysm phenotypes, which would suffer the most from the rigid wall assumption when modelling the pathology.

Discussion. The few publications reporting FSI simulation results for IAs investigate complex patient-specific geometries and employ a broad spectrum of physical parameters. The influence of these parameters on the obtained results has barely been assessed, although publications have reported that IAs may demonstrate a wide range of mechanical properties and thickness profiles, due to biological phenomena associated with their formation and growth [4]. Although the analysis of patient-specific aneurysms stands as our ultimate research goal, we think that simple trends have to be underlined on rudimentary test cases such as the one introduced here in order to get a better comprehension of the FSI modelling relevance.

REFERENCES

[1] Torii, R. et al. Fluid–structure interaction modeling of a patient-specific cerebral aneurysm: influence of structural modeling. *Comput Mech* **43**, 151–159 (2008).

[2] Ramalho, S. et al. Influence of Blood Rheology and Outflow Boundary Conditions in Numerical Simulations of Cerebral Aneurysms. In: Ledzewicz, U., Schättler, H., Friedman, A., Kashdan, E. (eds) Mathematical Methods and Models in Biomedicine (2013).

[3] Nemer, R. et al. Stabilized finite element method for incompressible solid dynamics using an updated Lagrangian formulation. *Computer Methods in Applied Mechanics and Engineering* **384** (2021).

[4] Meng, H. et al. High WSS or low WSS? Complex interactions of hemodynamics with intracranial aneurysm initiation, growth, and rupture: toward a unifying hypothesis. *AJNR* **35(7)**, 1254-62 (2014).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Development of a reduced-order model for understanding FL thrombosis in type B aortic dissection using a global sensitivity analysis and polynomial chaos expansion

Melito Gian Marco[1,*], Jafarinia Alireza[2,*], Müller Thomas Stephan[3], Rolf-Pissarczyk Malte[4], Holzapfel A. Gerhard[4], Brenn Günter[3], Hochrainer Thomas[2], Ellermann Katrin[1],

[1] Institute of Mechanics, Graz University of Technology, Austria; e-mail: gmelito@tugraz.at
[2] Institute of Strength of Materials, Graz University of Technology, Austria; email: alireza.jafarinia@tugraz.at
[3] Institute of Fluid Mechanics and Heat Transfer, Graz University of Technology, Austria
[4] Institute of Biomechanics, Graz University of Technology, Austria

Abstract: In this study, we focus on developing a reduced-order model to understand the most significant morphological parameters influencing FL thrombosis in Type B Aortic Dissection using a combination of the thrombus formation model and global sensitivity analysis. The results provide valuable insights into how various morphological parameters influence FL thrombosis. Additionally, by introducing non-dimensional parameters, we aim to enable the ability to transfer results between patients. The sensitive parameters identified in this study play a crucial role in classifying morphologies into a patent, a partially thrombosed, and a completely thrombosed FL. Specifically, a polynomial chaos expansion (PCE) is used to create a reduced-order model that can be used for further analysis and optimization, leading to a more efficient and accurate understanding of TBAD.

Keywords: Aortic dissection, Thrombus formation, Global sensitivity analysis, Morphological parametrization, Thrombus classification

1 Introduction

Type B aortic dissection (TBAD) is a relatively rare medical condition with a high mortality rate in which a tear in the intimal layer of the descending part of the aorta allows blood to flow between the layers of the aortic wall, causing them to separate. This creates a false lumen (FL) that originates in the descending aorta and may expand into the abdomen as the disease progresses. The FL can also extend into the thorax, leading to aortic regurgitation, myocardial ischemia, and even heart failure. In some cases, the FL can also extend into the aortic arch, leading to cerebral and spinal ischemia. In most cases, one or more 're-entry' tears form an additional path for blood flow between the true lumen (TL) and the FL. This creates a dynamic environment that can lead to an unstable and rapidly progressing dissection [1, 2].

Since TBAD is associated with late adverse events such as aortic rupture, rapid aortic growth, aneurysm formation, and organic and limb ischemia, it requires regular medical monitoring, which remains a challenge despite recent advances in clinical practice. A significant predictor for late dissection-related deaths and re-treatment of the descending aorta is the FL status, which refers to the amount of thrombus in the FL. The FL status is classified as patent (thrombus free), partially or completely thrombosed. A complete thrombosis in the FL can

slow down or stop the dissection progression, and it is associated with the lowest FL growth rates and the best outcomes in terms of survival and morbidity.

A global sensitivity analysis is applied to the FL thrombosis status computed in a parametrized 2D idealized aortic morphology. This analysis aims to determine the relative importance of the different input variables on the model output. A reduced-order model can be created that only includes the most significant variables by identifying the most sensitive variables. This reduced-order model can then be used for further analysis and optimization, leading to a more efficient and accurate understanding of TBAD. The sensitivity analysis is performed by formulating a surrogate model, such as the polynomial chaos expansion (PCE), that can be used to create a reduced-order model. The PCE is a mathematical technique that approximates the output of a computational model with a series of polynomials. This approach can be used to significantly reduce the computational cost of the model while preserving its accuracy [3, 4].

The sensitivity analysis revealed the most significant morphological parameters influencing FL thrombosis in TBAD. These results were used to classify morphologies based on the likelihood of developing a patent, partially or completely thrombosed FL. By using dimensionless numbers, we can transfer the results between patients, accounting for variations in aorta sizes and individual patient differences. The results can contribute to medical diagnostics and patient prognosis, helping accelerate prevention and therapy planning, especially for high-risk patients [5].

2 Acknowledgements

This work was funded by Graz University of Technology, Austria, through the LEAD Project on Mechanics, Modeling, and Simulation of Aortic Dissection.

References

[1] Nienaber CA, Clough RE, Sakalihasan N, Suzuki T, Gibbs R, Mussa F, Jenkins MP, Thompson MM, Evangelista A, Yeh JS, Cheshire N. Aortic dissection. Nature reviews Disease primers. 2016;2(1):1-8.

[2] Pepe A, Li J, Rolf-Pissarczyk M, Gsaxner C, Chen X, Holzapfel GA, Egger J. Detection, segmentation, simulation and visualization of aortic dissections: A review. Medical image analysis. 2020;65:101773.

[3] Saltelli A, Ratto M, Andres T, Campolongo F, Cariboni J, Gatelli D, Saisana M, Tarantola S. Global sensitivity analysis: the primer. John Wiley & Sons; 2008.

[4] B, Sudret. Global sensitivity analysis using polynomial chaos expansions. J Reliab Eng Syst Saf 2008; 93(7):964-979

[5] Jafarinia A, Melito GM, Müller TS, Rolf-Pissarczyk M, Holzapfel GA, Brenn G, Ellermann K, Hochrainer T. Morphological parameters affecting false lumen thrombosis following type B aortic dissection: a systematic study based on simulations of idealized models. Biomechanics and Modeling in Mechanobiology. 2023:1-20.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Chronic type B aortic dissection remodeling assessed with patient-specific fluid-structure interaction models

M. Rolf-Pissarczyk[1], K. Bäumler[2], R. Schussnig[3], T.-P. Fries[4], D. Fleischmann[2], A.L. Marsden[5], and G.A. Holzapfel[1,6]

[1] Institute of Biomechanics, Graz University of Technology, Austria, e-mail: m.rolf-pissarczyk@tugraz.at

[2] 3D and Quantitative Imaging Laboratory, Department of Radiology, Stanford University, CA, USA

[3] High-Performance Scientific Computing, University of Augsburg, Germany

[4] Institute of Structural Analysis, Graz University of Technology, Austria

[5] Department of Pediatrics and Bioengineering, Stanford University, CA, USA

[6] Department of Structural Engineering, Norwegian University of Science and Technology, Norway

Abstract: Aortic dissection is a life-threatening condition, characterized by the abrupt formation of a new parallel flow channel, the false lumen. Degeneration and aneurysm formation of the false lumen in the chronic phase of the disease are the main cause for late complications and death [Fleischmann, 2022]. The interplay between anatomic remodeling, hemodynamics and wall stress over the course of the disease are not yet well understood. We present a numerical framework to investigate the evolution of a patient's aortic dissection, captured by surveillance imaging with CTA from the subacute phase to five years after disease onset. Two-way fluid–structure interaction models are implemented in the open-source software SimVascular [Updegrove, 2016] allowing for the implementation of varying wall thicknesses, prestresses, external tissue support and anisotropic material properties of the dissected aorta [Rolf-Pissarczyk, 2021]. Aortic geometries, in vitro 4D flow MRI and the patient's blood pressure are used to then apply in vivo boundary conditions at each follow-up instance. This allows us to study the interplay between gradual deformation of the aorta and altered hemodynamics at different stages after the disease. Finally, the result's dependency on anisotropic material models describing the pathological microstructure of the aorta is examined by comparison with a simple isotropic model.

Keywords: Aortic dissection, hemodynamics, fluid-structure interaction

References:

[1] D. Fleischmann, R.O. Afifi, A.I. Casanegra, J.A. Elefteriades, T.G. Gleason, K. Hanneman, E.E. Roselli, M.J. Willemink, M.P. Fischbein et al.: *Imaging and surveillance of chronic aortic dissection: a scientific statement from the American Heart Association*, Circ Cardiovasc Imaging, 2022, 15:e000075.

[2] A. Updegrove, N.M. Wilson, J. Merkow, H. Lan, A.L. Marsden and S.C. Shadden: *SimVascular: an open source pipeline for cardiovascular simulation*, Ann Biomed Eng, 2016, 45:525–541.

[3] M. Rolf-Pissarczyk, K. Li, D. Fleischmann and G.A. Holzapfel: *A discrete approach for modeling degraded elastic fibers in aortic dissection*, Comput Methods Appl Mech Eng, 2021, 373:113511.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Accelerated Dirichlet-Robin fluid-structure interaction in patient-specific hemodynamics

R. Schussnig[1,2], **M. Rolf-Pissarczyk**[3], **K. Bäumler**[4], **G.A. Holzapfel**[3,5], **T.-P. Fries**[2] **and M. Kronbichler**[1]

[1] High Performance Scientific-Computing, University of Augsburg, Germany
e-mail: richard.schussnig@uni-a.de
[2] Institute of Structural Analysis, Graz University of Technology, Austria
[3] Institute of Biomechanics, Graz University of Technology, Austria
[4] 3D and Quantitative Imaging Laboratory, Department of Radiology, Stanford University, CA, USA
[5] Department of Structural Engineering, Norwegian University of Science and Technology, Norway

Abstract: Computational modeling of the cardiovascular system through fluid-structure interaction continues to pose challenges for numerical methods, since the involved incompressible continua are tightly coupled and exhibit complex material behavior. Here, we apply a semi-implicit fluid-structure interaction scheme [Schussnig et al., CMAME, 400:115489, 2022] in the context of aortic dissection. The combination of Robin transmission conditions and interface quasi-Newton methods accelerates and robustifies the partitioned coupling scheme, and allows detailed investigations of related biomarkers in a clinical setting.

Keywords: fluid-structure interaction, quasi-Newton method, Robin conditions, semi-implicit coupling

1 Introduction

Computational biomechanics has shown to be a particularly valuable tool for clinical support, as measurements on digital twins allow non-invasive investigations. However, increasingly rich models pose enormous challenges even for modern numerical tools, so that the development of suitable algorithms for clinical support is crucial. For this purpose, we employ a semi-implicit fluid-structure interaction (FSI) scheme [1, 2] that incorporates aspects like non-Newtonian rheology or outflow models related to volumetric flow rates and pressures. This allows us to analyze the role of relevant biomarkers such as time-averaged shear stresses and pressure differences on disease progression and long term outcomes.

2 Methods and results

A patient-specific aortic dissection dataset [3] is considered, creating a layered representation of the aortic wall and dissection flap separating the true and false lumen, as in Fig. 1(a). We adopt physiological parameters in Carreau fluid and HGO solid models [4]. With regard to the boundary conditions, we account for viscoelastic support on the exterior of the vessel, the downstream vasculature via Windkessel models and inflow data reconstructed from 4D MRI data [3]. After an initial precursor flow simulation has reached a periodic state, the fluid loads acting on the tissue are extracted and used to recover a prestress present at the time of medical imaging as in [2]. A semi-implicit FSI scheme with Robin interface conditions and quasi-Newton acceleration then couples fluid pressure and structural displacements in

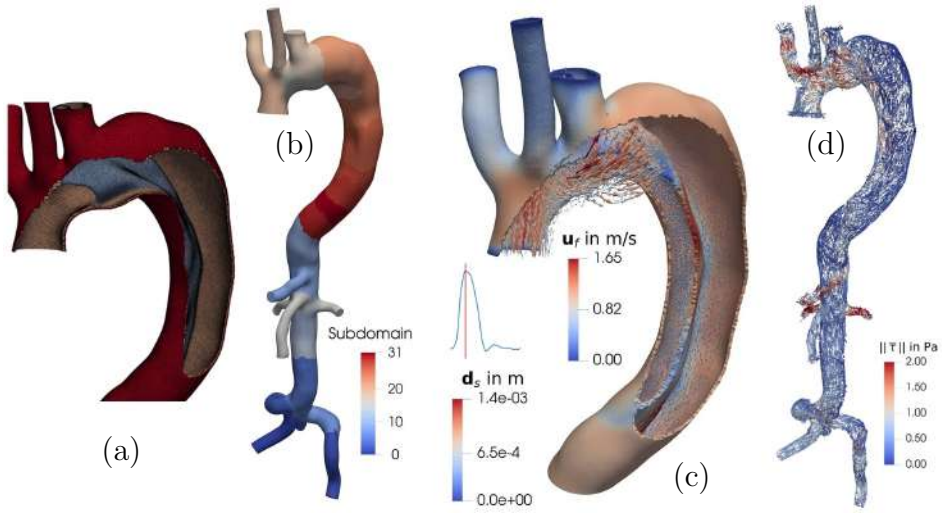


Figure 1: Aortic dissection case: cut tissue layers in aortic arch (a), partitioned domain (b), fluid velocity vectors $\boldsymbol{u}_f$ and solid displacement norm $\boldsymbol{d}_s$ at the peak systole of the fifth cardiac cycle (c) and time-averaged shear stress vectors $\bar{\boldsymbol{\tau}}$ at the fluid-structure interface (d).

an added-mass stable fashion. The fifth cardiac cycle solution is further analyzed by, e.g., inspecting flow splitting and pressure differences at peak systole or the time-averaged shear stresses, as shown in Figs. 1(c) and (d), which may be associated with further progression of the disease.

3 Concluding remarks

The proposed framework combines cardiovascular modeling with efficient methods for FSI and delivers promising first results. Ongoing work focuses on comparing various tissue and blood models, their effect on biomarkers and aspects of high-performance computing.

Acknowledgements. The authors thank TUGraz for financial support of the LEAD project *"Mechanics, Modeling and Simulation of Aortic dissection"* and the AI Production Network for support of RS.

References

[1] R. Schussnig, D.R.Q. Pacheco, and T.-P. Fries. Efficient split-step schemes for fluid-structure interaction involving incompressible generalised Newtonian flows. *Comput. Struct.*, 260:106718, 2022.

[2] R. Schussnig, D.R.Q. Pacheco, M. Kaltenbacher, and T.-P. Fries. Semi-implicit fluid-structure interaction in biomedical applications. *Comput. Methods Appl. Mech. Eng.*, 400:115489, 2022.

[3] K. Bäumler, V. Vedula, A.M. Sailer, J. Seo, P. Chiu, G. Mistelbauer, F.P. Chan, M.P. Fischbein, A.L. Marsden, and D. Fleischmann. Fluid-structure interaction simulations of patient-specific aortic dissection. *Biomech. Model. Mechanobiol.*, 19(5):1607–1628, 2020.

[4] G.A. Holzapfel, J.A. Niestrawska, R.W. Ogden, A.J. Reinisch, and A.J. Schriefl. Modelling non-symmetric collagen fibre dispersion in arterial walls. *J. R. Soc. Interface*, 12(106):20150188, 2015.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Image-based computational fluid dynamics of mitral regurgitation in the left heart

Bennati Lorenzo[1*], Giambruno Vincenzo[2], Renzi Francesca[1], Puppini Giovanni[3], Luciani Giovanni Battista[2] and Vergara Christian[4]

[1]Department of Surgery, Dentistry, Pediatrics, and Obstetrics/Gynecology
University of Verona, Verona, 37126, Italy
e-mail: lorenzo.bennati@univr.it, francesca.renzi@univr.it

[2]Division of Cardiac Surgery, Department of Surgery, Dentistry, Pediatrics,
and Obstetrics/Gynecology, University of Verona, Verona, 37126, Italy
email: vincenzo.giambruno@univr.it, giovanni.luciani@univr.it

[3]Department of Radiology, University of Verona, Verona, 37126, Italy
email: giovanni.puppini@aovr.veneto.it

[4]LaBS, Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta",
Politecnico di Milano, Milano, 20133, Italy
email: christian.vergara@polimi.it

Abstract: In this work we perform a computational study of the blood dynamics of the whole heartbeat in a patient with mitral valve regurgitation (MVR). To do this we use computational fluid dynamics (CFD) with prescribed motion of the left heart (LH) walls (left atrium, left ventricle and aortic root) and valves reconstructed from cine-MRI images. Our results highlight the presence of a regugitant jet in the left atrium leading to high WSS. Moreover, there is a large transition to turbulence, especially during the deceleration phase of the systolic ventricular blood flow.

Keywords: Cine-MRI, CFD, mitral valve regurgitation

1 Introduction

Mitral Valve Regurgitation (MVR) is the formation of a regurgitant flow in the left atrium due to an incomplete closure of the valve leaflets during the systolic phase. The knowledge of haemodynamic quantities such as velocity and Wall Shear Stresses (WSS) can help the surgeons to better understand the pathology and can be computed by means computational methods. In particular, we focus on Computational Fluid Dynamics (CFD) with imposed walls and valves motion where the displacement of the geometries is provided by kinetic medical images. Based on the available imaging, there are different approaches to reconstruct and prescribe the motion of the left heart (LH) walls and valves in CFD studies. For example, the majority of the CFD works used template geometries to include either the presence of the valves or of the left atrium (LA) and aortic root (AR).

The aim of this study aims to perform, for the first time at the best of our knowledge, a fully patient-specific image-based CFD simulation with imposed motion of the whole heartbeat on a patient with MVR by reconstructing the LH walls and valves from cine-MRI images.

2 Methods

To reconstruct the geometry and displacement of the LH walls, we combined two different reconstruction techniques for the left ventricle (LV) [1] and for the LA and AR, respectively. Registration of the LH displacement is performed through the non-affine B-splines algorithm implemented in the Elastix open source library (http://elastix.isi.uu.nl)

Concerning the valves, we reconstructed the patient-specific mitral valve (MV) in its fully open and fully closed configuration by using the method proposed in [1]. For the aortic valve, instead, we deformed a template geometry to match its annulus with the annulus detected from the cine-MRI images.

For CFD, we considered the Navier-Stokes equations written in a Arbitrary Lagrangian-Eulerian (ALE) framework with a LES model for transition to turbulence [2] and the Resistive Immersed Implicit Surface (RIIS) model to manage the valve dynamics [3].

3 Results

We found a large amount of transition to turbulence especially during the deceleration phase of the systolic ventricular flow. In particular, in Figure 1, we reported on the left the trend in time of the Global Turbulent Kinetic Energy (GTKE) calculated over 6 heartbeats. The maximum value is reached during the deceleration phase of the systolic ventricular flow. At this time instant, we showed, on the right, the ensemble velocity $\mathbf{u}$ and the Standard Deviation (SD) of the velocity fluctuations.

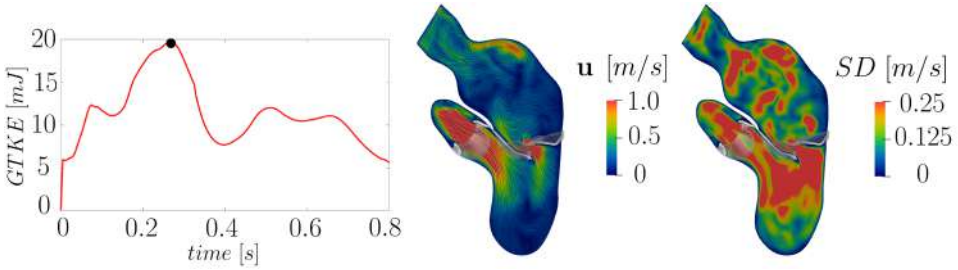


Figure 1: Left: trend in time of GTKE. Right: ensemble velocity (left) and SD of the velocity fluctuations (right) at the time instant of maximum GTKE.

References

[1] Bennati, L. et al. An image-based computational fluid dynamics study of mitral regurgitation in presence of prolapse. MOX Rep. n* 18/2022, Dipartimento di Matematica, Politecnico di Milano, 2022.

[2] Nicoud, F et al. Using singular values to build a subgrid-scale model for large eddy simulation. Phys. Fluids - PHYS FLUIDS 23, 2011.

[3] Fedele, M et al. A. A patient-specific aortic valve model based on moving resistive immersed implicit surfaces. Biomech. modeling mechanobiology 16, 1779–1803, 2017. (2017).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Unified continuum fluid-structure interaction simulation of treatment for mitral regurgitation

Joel Kronborg* **and Johan Hoffman***

* Department of Computer Science
KTH Royal Institute of Technology
Stockholm, Sweden
e-mail: joelkro@kth.se, jhoffman@kth.se

Abstract: Mitral regurgitation is a serious heart condition in which the mitral valve, located between the left atrium and the left ventricle in the heart, does not close properly when the heart contracts. A minimally invasive treatment method for this is by using a mitral valve clip to permanently close off part of the valve. We simulate the outcome of this type of treatment, with the goal to give heart surgeons predictions of the outcome of the surgery and help them make better informed treatment decisions. To this end, we use a patient-specific model of the left ventricle, combined with a fluid-structure interaction model of the mitral valve. The model uses an arbitrary Lagrangian-Eulerian finite element method on a monolithic mesh. To evaluate and improve the model, we apply it to patient-specific data from mitral regurgitation patients at Karolinska Hospital in Stockholm, Sweden. Here we present the current progress of the work.

Keywords: Fluid-structure interaction, Mitral valve, Mitral regurgitation, Patient-specific heart modelling

1 Introduction

Treatment for mitral regurgitation is often done by using a mitral valve (MV) clip. This is a minimally invasive procedure, which is especially advantageous for patients at high surgical risk. Computer simulations have shown promise in predicting the outcome of the procedure[1]. In a recent study, we simulated intraventricular blood flow after a mitral valve clip procedure in a patient-specific model of the left ventricle (LV)[2]. We used a planar model of the MV, corresponding to a projection of the valve leaflets onto the ventricle wall. In a separate study, we simulated blood flow in an idealized model of the aortic valve (AV), using a unified continuum (UC) fluid-structure interaction (FSI) approach[3]. To improve the LV simulation of the MV clip procedure, we now apply the same UC-FSI method to simulate the MV leaflets.

2 Method

Our patient-specific model of the LV is created from transthoracic echocardiography (TTE) images[4]. The LV wall is segmented in the images at snapshots over the entire heart beat cycle, and surface meshes are generated throughout the cycle. These are then used to generate a deforming volume mesh. During simulation the snapshot meshes are interpolated to simulate the valve wall movement throughout the heart beat cycle.

The UC-FSI approach, which we used previously for the AV, and now for the MV, uses a monolithic mesh, with the solid and fluid parts marked as separate subdomains. To simulate

the blood flow, an arbitrary Lagrangian-Eulerian (ALE) finite element method (FEM) is used, effectively simulating the fluid flow as Eulerian, but on a moving mesh where the motion of the leaflets is simulated in a Lagrangian sense. Two mesh smoothing algorithms are used to handle the deformation of the mesh: one using Laplacian smoothing, and one an elastic analogy. Contact between the leaflet tips is simulated by marking a subdomain of the fluid region as a contact region. When the distance between the leaflet tips is small, the contact region switches from fluid state to solid, effectively closing off the valve opening temporarily.

Simulating FSI in this manner has several advantages. By using a monolithic mesh, no mapping has to be done between separate solid and fluid meshes, eliminating the risk of introducing errors from this. Additionally, the entire simulation can be solved as one unified system. By using the contact region to simulate contact between the leaflets, the leaflet tips can be kept separated enough so that the mesh cells between them do not collapse. Thereby, the simulation can be done without remeshing during run time, again eliminating potential errors in mapping between meshes. However, meshing has to be done carefully to ensure satisfactory spatial resolution when the valve is fully open, while also not running a high risk of mesh collapse when the valve closes.

3 Results

Work is still ongoing to develop the FSI model of the MV. Results from simulations of blood flow after MV clip treatment with the planar valve model show a significant increase in shear in the intraventricular blood flow after treatment, which could indicate an elevated risk of thrombosis formation downstream[2].

References

[1] Caballero A, Mao W, McKay R, Hahn RT and Sun W. A comprehensive engineering analysis of left heart dynamics after MitraClip in a functional mitral regurgitation patient. Frontiers in Physiology; 2020, 11, p. 432.

[2] Kronborg J, Svelander F, Eriksson-Lidbrink S, Lindström L, Homs-Pons C, Lucor D and Hoffman J. Computational analysis of flow structures in turbulent ventricular blood flow associated with mitral valve intervention. Frontiers in Physiology; 2022, p. 752.

[3] Hiromi Spühler J and Hoffman J. An interface-tracking unified continuum model for fluid-structure interaction with topology change and full-friction contact with application to aortic valves. International Journal for Numerical Methods in Engineering; 2021, 122, p. 5258–5278.

[4] Larsson D, Hiromi Spühler J, Petersson S, Nordenfur T, Colarieti-Tosti M, Hoffman J, Winter R and Larsson M. Patient-specific left ventricular flow simulations from transthoracic echocardiography: robustness evaluation and validation against ultrasound Doppler and magnetic resonance imaging. IEEE transactions on medical imaging; 2017, 36, p. 2261–2275.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Patient-Specific Image-Based Computational Fluid Dynamic Model of the Right Heart

Renzi Francesca[1*], Fedele Marco[2], Giambruno Vincenzo[3], Quarteroni Alfio[2,4], Puppini Giovanni[5], Luciani Giovanni Battista [3], Vergara Christian[6]

[1*] Department of Surgery, Dentistry, Pediatrics, and Obstetrics/Gynecology
University of Verona, Verona, Italy
e-mail: francesca.renzi@univr.it

[2] MOX, Department of Mathematics
Politecnico di Milano, Milano, Italy
e-mail: marco.fedele@polimi.it, alfio.quarteroni@polimi.it

[3] Division of Cardiac Surgery, Department of Surgery, Dentistry, Pediatrics, and Obstetrics/Gynecology
University of Verona, Verona, Italy
email: vincenzo.giambruno@univr.it, giovanni.luciani@univr.it

[4] Ecole Polytechnique Fédérale de Lausanne
Rte Cantonale, Lausanne, Switzerland

[5] Department of Radiology
University of Verona, Verona, Italy
email: giovanni.puppini@aovr.veneto.it

[6] LaBS, Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta"
Politecnico di Milano, Milano, Italy
email: christian.vergara@polimi.it

Abstract: Clinical interest in the right side of the heart (RH) has increased significantly due to the awareness of its relevance in acquired and congenital heart diseases. In this work, we aim at improving the RH knowledge by developing patient-specific Computational Fluid Dynamics (CFD) models of the complete RH of a healthy subject and a patient with tetralogy of Fallot. In this regard, we present a novel method for the reconstruction of the RH geometry and displacement starting from cine-MRI, suitable for CFD simulations with prescribed motion.

Keywords: Right heart, cine-MRI, image registration, CFD

1 Introduction

Changes in right cardiac structure and function have prognostic implications in several congenital and acquired heart diseases, such as Tetralogy of Fallot (ToF) or pulmonary hypertension. For this reason, the study of the Right Heart (RH) function is of utmost relevance in clinical practice[1].

Blood dynamics is affected by many of such diseases and Computational Fluid Dynamics (CFD) models are proven to be valid tools for the quantitative and non-invasive analysis of blood pressures, velocities, and wall shear stresses, which is crucial to improve the understanding of the RH function. To the best of the authors' knowledge, the literature lacks

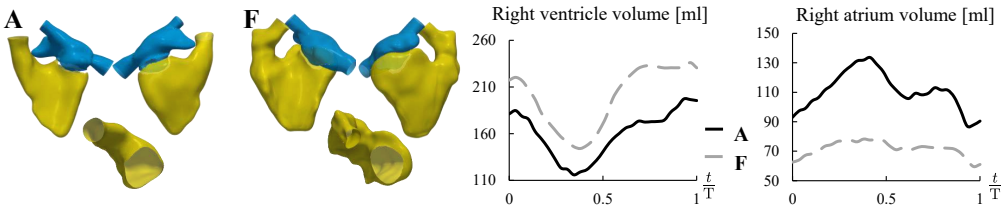


Figure 1: Left: RH reconstruction of a healthy subject (A) and a ToF patient (F). Right: volume curves of right ventricle and atrium over the time frames of a heartbeat.

CFD models of the complete beating RH, including both the atrium and the ventricle.

In this work, we aim to develop a complete patient-specific RH CFD model where the wall displacement is reconstructed from images by means of a novel reconstruction method based only on cine-MRI.

2 Methods

To reconstruct the geometry and displacement of the RH we developed a novel method that is able to merge the information coming from different MR acquisition series and requires minimal user contribution. After the manual tracing of the endocardium on the cine-MRI slices for a specific time frame, the method automatically contours the endocardium for the remaining frames of the heartbeat, exploiting image registration techniques. From these contours, the endocardial surface is reconstructed at each frame by morphing a template surface. Finally, the 3D endocardial displacement is obtained through a non-rigid B-spline-based registration algorithm among level-set images (`http://elastix.isi.uu.nl`).

On the reconstructed RH geometries we performed CFD simulations using the C++ library `lifex`[2], solving the Navier-Stokes equations in an Arbitrary Lagrangian-Eulerian framework where the domain moves according to the reconstructed displacement field.

3 Results

We built the RH models of a healthy subject and a patient with repaired ToF, represented in Fig. 1, with the proposed reconstruction method. We assessed the accuracy of the method by comparing the resulting reconstructions with the patient's cine-MRI. Moreover, we analyzed the robustness of the method by varying the amount of cine-MRI acquisition series used for the RH reconstruction of a specific subject. Finally, we analyzed the CFD results obtained in the reconstructed geometries to assess the reliability of our method to answer specific clinical questions.

References

[1] Domitrescu S I, Tintoiu I C, Underwood M J. Right heart pathology: from mechanism to management. Springer, 2018.

[2] Africa PC. lifex: A flexible, high performance library for the numerical solution of complex finite element problems. SoftwareX 20, 2022 Dec, 101252.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Computational hemodynamics and fluid-structure interaction for native and prosthetic cardiac valves

Fumagalli Ivan[*,1], **Renzi Francesca**[2], **Polidori Rebecca**[3], **Dacatra Eleonora S.**[4], **Dede' Luca**[1], **Vergara Christian**[4], **Quarteroni Alfio**[1,5]

[1] MOX - Dipartimento di Matematica
Politecnico di Milano
Milan, Italy
e-mail: ivan.fumagalli@polimi.it

[2] Dipartimento di Scienze Chirurgiche Odontostomatologiche e Materno-Infantili
Università di Verona
Verona, Italy

[3] Dipartimento di Biotecnologie mediche e Medicina traslazionale
Università degli Studi di Milano
Milano, Italy

[4] LaBS – Dipartimento Di Chimica, Materiali e Ingegneria Chimica
Politecnico di Milano
Milan, Italy

[5] Mathematics Institute
École Polytechnique Fédérale de Lausanne
Lausanne, Switzerland

Abstract: In the investigation of cardiac hemodynamics, the reconstruction of the geometry and motion of the valves is often very difficult, due to the small thickness of the leaflets and their fast dynamics. Therefore, computational models for valves are often required. These models range from prescribed-displacement computational fluid dynamics - with the valve opening/closing triggered by local measures of pressures or flow rate - to three-dimensional Fluid-Structure Interaction (FSI). The choice of the model depends on available resources, required response time, and clinical question of interest. In this talk, we present computational methods used to answer specific clinical questions related to prosthetic valves. In particular, we focus on identifying prediction factors for the degeneration of a transcatheter aortic valve and assessing the hemodynamics of a prosthetic pulmonary valve, in patient-specific geometries. In these applications, we employ 3D FSI and/or a reduced multiscale FSI system entailing a lumped-parameter model for the valve dynamics. We then discuss and compare the level of detail and the computational efficiency of the different methods.

Keywords: CFD, FSI, cardiac valve modeling, transcatheter aortic valve implantation

1 Introduction

Many cardiac diseases are related to valve dysfunctions, for whose treatment the implantation of a valve prosthesis is very often preferred to surgical repairment. In this talk, we present different computational models for the interaction between prosthetic valve dynamics and blood flow, as well as their application to two clinical problems: a study on the degeneration of a Transcather Aortic Valve Implantation (TAVI) device for the treatment of Aortic Valve

Stenosis (AVS) [1], and the assessment of a Self-Expandable Pulmonary Valve (SEPV) for the treatment of pulmonary regurgitation in repaired-Tetralogy-of-Fallot (rToF) patients.

2 Models and methods

The computational domain of interest is either the ascending aorta (in the case of the TAVI) or the main pulmonary arteries (in the case of the SEPV), reconstructed from CT scans. The blood flow is modeled by incompressible Navier-Stokes equations. The prosthesis stent is modeled as a linear elastic solid, whose dynamics is coupled with the flow in a fully 3D Fluid-Structure Interaction (FSI) system with an arbitrary Lagrangian-Eulerian formulation of the fluid problem. For the leaflets, we adapt a lumped-parameter model originally developed for the native aortic valve [2] and hinging upon a Resistive Immersed Implicit Surface (RIIS) [3] representation of the leaflets, resulting in a reduced 3D-0D FSI model. These methods are implemented in the multi-physics finite element library `lifex` (https://lifex.gitlab.io/) [4].

3 Results and discussion

Using the models described above, we could investigate the hemodynamics of different TAVI patients and find preliminary predictive indicators correlating with the structural degeneration of the prosthetic leaflets. The extension of the model to the case of the SEPV showed how this prosthesis is effective in recovering a physiological pulmonary flow in rToF patients. The reduced leaflet model is proven to be flexible enough to represent the rather different dynamics associated with a native AV (both physiological and stenotic), a prosthetic AV, and a SEPV, requiring only parameter calibration.

Acknowledgements

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 740132, IHEART 2017-2022, P.I. A. Quarteroni).

References

[1] Fumagalli I, Polidori R, Renzi R, Fusini L, Quarteroni A, Pontone G, Vergara C. Fluid-structure interaction analysis of transcatheter aortic valve implantation. MOX report 29/2022; 2022.

[2] Fumagalli I. A reduced 3D-0D FSI model of the aortic valve including leaflets curvature. MOX report 30/2021; arXiv:2106.00571 [math.NA]; 2021.

[3] M. Fedele, E. Faggiano, L. Dedé, A. Quarteroni, A patient-specific aortic valve model based on moving resistive immersed implicit surfaces. Biomech Model Mechan 2017;16(5):1779-1803.

[4] Africa, P.C. `lifex`: a flexible, high performance library for the numerical solution of complex finite element problems. SoftwareX, 2022;20:101252.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Predicting left atrium stasis patterns from a data-augmented patient-specific geometry database in atrial fibrillation conditions

Jorge Dueñas-Pamplona[*†], Javier García[†], José Sierra-Pallares[††], Conrado Ferrera[†††], and Francisco Castro[††]

[†] Departamento de Ingeniería Energética
Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid
Madrid, Spain
[*] e-mail: jorge.duenas.pamplona@upm.es

[††] Departamento de Ingeniería Energética y Fluidomecánica
Escuela de Ingenierías Industriales, Universidad de Valladolid
Valladolid, Spain

[†††] Departamento de Ingeniería Mecánica, Energética y de los Materiales
Escuela de Ingenierías Industriales, Universidad de Extremadura
Badajoz, Spain

Abstract: During recent years, advances in medical imaging, segmentation techniques, and high-performance computing are paving the way to apply computational fluid dynamics (CFD) simulations to study the cardiovascular system, providing interesting insights to understand flow behaviour, both in physiological and pathological conditions. This is the case with atrial fibrillation (AF), which is the most common cardiac arrythmia. During an episode of AF, the beating of the left atrium (LA) becomes fast and irregular, increasing the risk of thrombus formation, and thus also the risk of stroke if one of these thrombi manages to reach the brain. Although the left atrial appendage (LAA) is the most common site of intracardiac thrombosis, the mechanical relationship between LA anatomy, flow patterns, and thrombus formation is still elusive. The aim of this work is to further explore this relationship, contrasting a range of geometrical and flow parameters that are known to affect LAA blood stasis and the 'dead volume' of blood that is formed within LAA under AF conditions. For this purpose, an in-house computational framework to perform cardiac parametric studies has been used, feeding simulation results from different patients into a data-driven model capable of predicting dead volume.

Keywords: atrial fibrillation, computational fluid dynamics, patient-specific modelling, data-driven modelling, left atrium

1. Introduction

Recent advances in medical imaging, segmentation techniques, and high-performance computing have boosted the use of patient-specific computational fluid dynamics (CFD) simulations. This has provided important insights to understand the mechanism of diseases such as atrial fibrillation (AF) [1], which triggers fast and irregular beatings, which are known to be associated with an increased risk of thrombosis.

Although it is known that LA and LAA morphologies contribute to LAA blood stasis and thrombosis, and the impact of LA anatomy and function on LAA hemodynamics is being further investigated [2], the mechanistic relationship between geometric parameters and blood stasis remains unknown.

To fill this gap, we performed a parametric study based on data-augmentation to increase the size of the geometry database, performing a series of CFD simulations which allowed us to identify common stasis patterns while applying morphological variations to patient-specific

geometries and determining how the geometric LA parameters are associated with stasis patterns.

2. Materials and Methods

Atrial CT images of several cardiac patients have been segmented, allowing us to reconstruct 3D patient-specific atrial geometries. After that, a data-augmentation procedure has been performed, allowing us to generate a larger synthetic geometry database from these initial patient-specific geometries. This was achieved by applying a morphing methodology [3], based on the rigging and skinning of each of the patient-specific geometries. This procedure allowed us to provide each geometry with an armature, designed to apply plausible variations of a range of selected geometry parameters: LAA volume, LAA ostium area, main LAA bend, number of lobes, etc.

An in-house computational framework to perform cardiac parametric studies has been used to simulate the synthetic geometries, performing parametric simulations and calculating the dead volume based on the M4 index [3] between others.

3. Discussion and Conclusions

We present a parametric study based on atrial geometry data-augmentation starting from patient-specific geometries. This approach could make it possible to avoid one of the major difficulties encountered in computational studies of this type, namely the lack of sufficient clinical data to ensure the generality of the simulation results. It also allowed us to quantify dead volumes by applying geometrical variations across various patient-specific geometries, illustrating some interesting features associated with blood stasis and thus related to thrombi formation.

Acknowledgements

This work was supported by the 'Ministerio de Ciencia, Innovación y Universidades' of Spain under the **DPI2017-83911-R** contract, and by the 'Junta de Extremadura' under the **IB20105** contract (partially financed by FEDER funds). The 'Programa Propio de la Universidad Politécnica de Madrid', the 'Ayuda Primeros Proyectos de Investigación ETSII-UPM', and the 'Programa de Excelencia para el Profesorado Universitario de la Comunidad de Madrid' are acknowledged.

References

[1] Zingaro A, Menghini F, Quarteroni A. Hemodynamics of the heart's left atrium based on a Variational Multiscale-LES numerical method. Eur. J. Mech. B Fluids. 2021;89:380-400.

[2] García-Villalba M, Rossini L, Gonzalo A, Vigneault D, Martinez-Legazpi P, Durán E, Flores O, Bermejo J, McVeigh E, Kahn AM, Del Álamo JC. Demonstration of patient-specific simulations to assess left atrial appendage thrombogenesis risk. Front. physiol. 2021;12:596596.

[3] Dueñas-Pamplona J, García J, Castro F, Muñoz-Paniagua J, Goicolea J, Sierra-Pallares J. Morphing the left atrium geometry: A deeper insight into blood stasis within the left atrial appendage. Appl. Math. Model. 2022;108:27-45.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modeling of stented arteries using mixed-dimensional interaction

Ivo Steinbrecher*, Nora Hagmeyer* and Alexander Popp*

* Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: ivo.steinbrecher@unibw.de

Abstract: Modeling stents based on 1-dimensional Cosserat continua (beam theory) is a promising approach to reduce the complexity of the numerical model. This introduces the need for mixed-dimensional interaction methods between the 1-dimensional stent model and the surrounding (higher-dimensional) structures. State of the art interaction methods are used to model a stented artery subject to a pressure wave. The resulting model is able to capture relevant effects such as the stiffening effect of the stent on the artery.

Keywords: Cardiovascular simulation, geometrically exact beam theory, mixed-dimensional interaction, finite element method

1 Introduction

Cardiovascular diseases represent one of the leading causes of death worldwide. This motivates the desire for minimally invasive stenting procedures, however, complications such as leakage, migration, restenosis, etc. frequently necessitates follow-up surgeries. Thus a computational tool to enhance the understanding of the procedure is desirable. Computational simulation of such biomedical problems are rather complex and necessitate large system sizes to adequately capture important phenomena. Motivated by the research of Tambača et al., cf. [1], who utilized the benefits of 1-dimensional beam theory to efficiently simulate the behavior of coronary stents and observed a good agreement with full-dimensional models at a fraction of the system size, we follow the concept of modeling stents using geometrically exact beam theory.

2 Mixed-dimensional modeling of a stented artery

Recent developments on mixed-dimensional coupling methods allow for an efficient and accurate coupling between 1-dimensional Cosserat continua (based on the geometrically exact beam theory) and higher dimensional objects (e.g., volumes or surfaces), see for example [2]. The so-called beam-to-solid/surface coupling methods are very efficient from a numerical point of view and yield accurate solutions. To study the applicability of such methods to model a stented artery, we set up a variant of the well-known fluid-structure interaction (FSI) benchmark problem of a pressure wave traveling through an elastic tube. This problem was originally proposed to validate the suitability of FSI algorithms for blood flow simulations. In addition to the original problem, we use the beam-to-surface coupling method to capture the effect of a diamond-shaped stent structure on the behavior of the overall system.

The results, which will be presented in the talk, show that the proposed model is capable of capturing the large change in compliance between the stented and unstented regions of the artery, thus leading to stress peaks in these transitional regions. Exemplarily, Figure 1(left) illustrates a snapshot of the problem right before the pressure wave reaches the stented region. Figure 1(right) shows the interaction forces between the stent and the artery wall. This example demonstrates the ability of mixed-dimensional coupling approaches to capture important phenomena, such as changes in compliance as well as the distribution of the interaction forces.

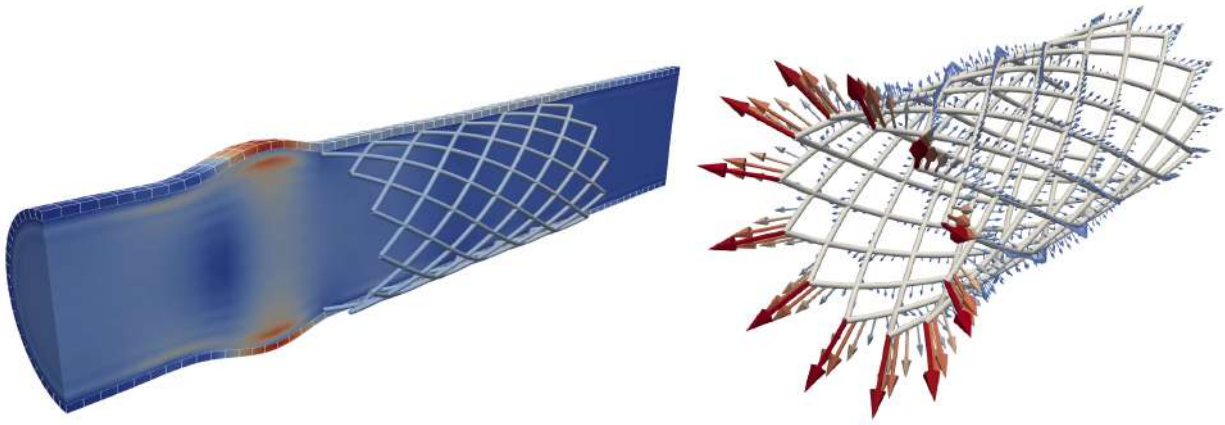


Figure 1: Illustrations of the stented artery. (left) The deformed configuration before the pressure wave reaches the stented region. (right) Interaction foces between the stent and the artery wall.

3 Conclusions

One of the topics that will be addressed in this talk is the employed mixed-dimensional modeling framework and how it can be used to model cardiovascular applications. Furthermore, the results of the problem described in the previous section will be presented in detail. Finally, possible future extensions to the proposed modeling approach and applications will be outlined.

References

[1] Tambača, J., Kosor, M., Čanić, S., D. Paniagua, M.D.: Mathematical modeling of vascular stents. SIAM Journal on Applied Mathematics **70**(6), 1922–1952 (2010)

[2] Steinbrecher, I., Hagmeyer, N., Meier, C., Popp, A.: A consistent mixed-dimensional coupling approach for 1D Cosserat beams and 2D solid surfaces (2022). Preprint, https://arxiv.org/abs/2210.16010

[3] Hagmeyer, N., Mayr, M., Steinbrecher, I., Popp, A.: One-way coupled fluid-beam interaction: capturing the effect of embedded slender bodies on global fluid flow and vice versa. Advanced Modeling and Simulation in Engineering Sciences **9**(1), 9 (2022)

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Sensitivity analysis and parameter estimation of a lumped parameter cardiovascular model during extracorporeal life support

Jan-Niklas Thiel*, Ana M. Costa†, Bettina Wiegmann‡, Jutta Arens† and Michael Neidlin*

* Department of Cardiovascular Engineering, Institute of Applied Medical Engineering
Helmholtz Institute, RWTH Aachen University, Aachen, Germany
e-mail: thiel@ame.rwth-aachen.de

† Department of Biomechanical Engineering, Engineering Organ Support Technologies Group
University of Twente, Enschede, Netherlands

‡ Department of Cardiothoracic, Transplantation and Vascular Surgery and Lower Saxony Center of Biomedical Engineering, Implant Research and Development (NIFE) and German Center for Lung Research (DZL), BREATH, Hannover Medical School, Hannover, Germany

Abstract: In this study a cardiovascular model including veno-venous extracorporeal membrane oxygenation (VV-ECMO) was developed to investigate patient-device interaction. Global Sensitivity Analysis (GSA) was performed to identify the two most crucial model parameters for each output. These parameters were subsequently used for fitting the model to patient data. The best fitting algorithm was used to show the quality of the fit. This study provides a basis for applying the model to patients receiving combined lung and kidney support, as well as larger patient cohorts.

Keywords: LPM, ECMO, AKI, CRRT, patient-device interaction, GSA, Sobol, parameter estimation

1 Introduction

ECMO is commonly used in intensive care to support cardiac and respiratory failure, yet up to 70% of these patients also suffer from acute kidney injury. The treatment for this complication, which involves connecting continuous renal replacement therapy (CRRT) to the ECMO circuit, lacks a gold standard and its connection configuration varies depending on the operator's practice and proficiency. Long term aim of this study is to develop a cardiopulmonary model to investigate the effect of different CRRT connection schemes on large ECMO cohorts. As a first step, this abstract focuses on the application to a VV-ECMO patient. A GSA using Sobol indices is conducted to identify most crucial model parameters for fitting, reducing the number of function evaluations (NFE) and thus its computational cost. Different solvers are compared with regard to performance and quality of the results.

2 Methodology

A computational cardiovascular model has been extended by a pulmonary system and an ECMO system with an external pump, oxygenator, and additional cannulae. This model was fitted to an ARDS patient with Influenza A Pneumonia (f, 28y, sedated) using different state-of-the-art solvers. A GSA was conducted using the Sobol method to identify the model parameters most relevant for the fitting. The Saltelli extension of the Sobol sequence was used to generate 512 samples that served as inputs for the GSA.

3 Results and Conclusions

Left part of Figure 1 shows the Total Sensitivity Index, which measures the total effect of each model parameter on the output of the system, including interactions between them. Model fitting was performed using the intersection of the two most important parameters for each output. These parameters were *Rsart*, *Rpart*, *Cpart*, *Rcanin*, *Roxy*, *Rcanout*, and *Emaxlv*.

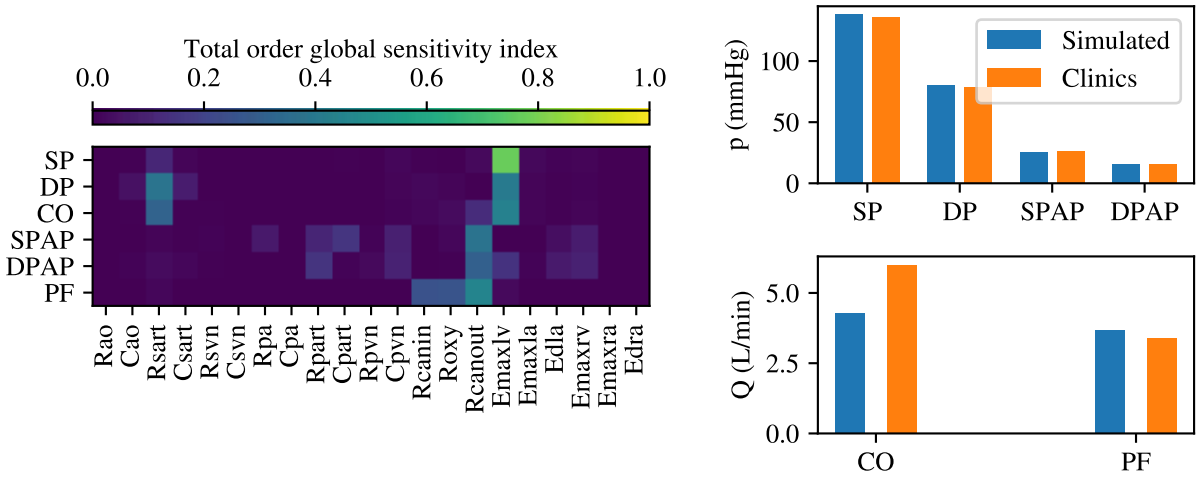


Figure 1: Left: total effect of each model parameter on the outputs. Right: comparison of model output for fitted model parameters. *R* and *C* represent resistances and compliances of model compartments, and *Emaxlv* is the elastance of the left ventricle. *SP*, *DP*, *SPAP*, *DPAP*: systolic and diastolic pressure of the aorta and the pulmonary arteries. *CO*: cardiac output. *PF*: pump flow.

Table 1 shows the results of different solvers for minimizing RMS error between simulated and clinical data, as well as the NFE required for convergence. The Sequential Least Squares Programming *SLSQP* algorithm was chosen for its low error value and computational cost. Its results are compared to clinical data on the right of Figure 1.

Table 1: Error and NFE for different solver.

Solver	Nelder-Mead	Powell	CG	BFGS	L-BFGS-B	CYBOLA	SLSQP
Error	0.022	0.020	0.11	0.31	0.020	0.047	0.019
NFE	569	2861	189	96	72	500	173

In summary, a cardiovascular model including VV-ECMO was analyzed using GSA, which revealed that fitting the model using only a subset of important model parameters reduces computational cost while maintaining the quality of the fit. This generic framework can now be extended to a more comprehensive model that incorporates different CRRT strategies and phenotypes from larger patient cohorts.

4 Acknowledgements

This project is funded by the DFG SPP2014 “Towards the Artificial Lung” - PN: 447746988.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Physiological Control Mechanisms in the Fontan Circulation

Ahmad, Zan[1,2], Puelz, Charles[2,3] and Peskin, Charles[2]

[1] Department of Applied Mathematics and Statistics
Johns Hopkins University
Baltimore, MD, USA
e-mail: zahmad6@jhu.edu

[2] Courant Institute of Mathematical Sciences
New York University
New York, NY, USA
e-mail: peskin@cims.nyu.edu

[3] Division of Pediatrics, Section of Cardiology
Baylor College of Medicine
Houston, TX, USA
e-mail: charles.puelz@bcm.edu

Abstract: Circulation models often treat heart rate as a given parameter. Here, we allow the heart rate to be continuously variable, and we model some of the feedback control mechanisms that influence the heart rate. These include the effects of systemic arterial pressure (which acts through a feedback loop involving the nervous system) and right atrial pressure (which acts directly on the cardiac pacemaker). We use our formulation to examine the effects of exercise on a normal physiology as well as a single ventricle physiology known as the Fontan circulation. In particular, we study the effect of control on the Fontan circulation by comparison to results obtained with an uncontrolled model in our previous work. We examine the dynamic effects of the introduction of a surgical modification (fenestration) to the Fontan physiology using our feedback control method. The controlled model more accurately justifies the optimized fenestration in the Fontan circulation. Additionally, we present comparisons between the hemodynamics during exercise in the normal circulation, Fontan circulation, and optimally fenestrated Fontan physiology.

Keywords: cardiovascular models, feedback control, Fontan circulation

1 Introduction

The Fontan circulation is a single-ventricle physiology surgically constructed to treat congenital heart defects. In a previous paper, we studied the effects of a fenestration between the systemic and pulmonary veins typically used to improve hemodynamics in Fontan patients [1]. This model was uncontrolled in the sense that heart rate was fixed, and thus had limitations simulating dynamic processes such as exercise. In this presentation, heart rate will be modeled as a continuously variable function depending on several physiological control mechanisms. The effects of exercise and surgical modifications to the Fontan circulation will be compared between the controlled and uncontrolled model. The control model will also be used to simulate the hemodynamic effects immediately after the opening of the fenestration. The following section simply describes the general method we will be using to solve for heart rate with an arbitrary control mechanism. Our results (reserved for presentation) will focus on the following two control mechanisms: systemic arterial pressure and right atrial pressure.

1.1 Equations

The following mathematical description allows heart rate, F, to be a continuously variable function in our model: Let $C_0(t_0)$ denote a ventricular compliance function which is periodic, with fixed period T_0 corresponding to a fixed heart rate parameter $F_0 = 1/T_0$. To produce a continuously variable heart rate, $F(t)$, we set the true compliance C to be

$$C(t) = C_0(t_0(t)) \tag{1}$$

where $t_0(t)$ satisfies the differential equation:

$$\frac{\mathrm{d}t_0}{\mathrm{d}t} = \frac{F(t)}{F_0} \tag{2}$$

Given $F(t)$, we solve (2) numerically, and then at each time step with t_0 known, we evaluate (1) by calling the function C_0 with its argument being the current value of t_0.

Then, we define F(t) as follows:

$$F(t) = F_0 + \Delta F \tag{3}$$

$$\Delta F = cF_0 \frac{P_{\text{filtered}} - P^*}{P^*} \tag{4}$$

where $c < 0$ and P^* is the set pressure value. Thus, F is a function of the deviation in certain pressure values known to regulate heart rate. The way that we define P^* depends on the type of perturbation we are considering. For example, during exercise, we obtain the most accurate results when we keep P^* equal to the mean systemic arterial pressure before exercise and slowly increase it as exercise begans. We use this to study the effects of parameter perturbations on the normal circulation, Fontan circulation and fenestrated Fontan in a zero-dimensional pulsatile model.

2 Conclusions

Traditionally, zero dimensional pulsatile blood flow models have heart rate as a known parameter, restricting their capabilities when dynamic perturbations need to be considered, such as exercise. It can clearly be seen from our formulations that the changes in P (either right atrial pressure or systemic arterial pressure) will accurately result in the appropriate update on the value of heart rate $F(t)$. A drop in either of these pressures will be detected by the controller as a deviation from the set value result in an increase in F and vise-versa. We use this method to study and compare the hemodynamics of the Fontan physiology during exercise in the controlled, uncontrolled, open fenestration and closed fenestration cases.

References

[1] Ahmad, Zan, et al. Optimal fenestration of the Fontan circulation. Frontiers in Physiology 13 (2022): 867995.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A multi-scale hybrid reduced order model for cardiovascular applications

Siena Pierfrancesco*, Gossard Audrey*, Girfoglio Michele* and Rozza Gianluigi*

* mathLab, Mathematics Area, SISSA, International School for Advanced Studies,
via Bonomea 265, I-34136 Trieste, Italy
e-mail: psiena@sissa.it, agossard@sissa.it, mgirfogl@sissa.it, grozza@sissa.it

Abstract: Cardiovascular diseases represent a crucial research topic, as a consequence of their diffusion worldwide. Due to the large computational cost of classic numerical models, an hybrid (data driven/Galerkin projection) Reduced Order Model (ROM) is developed in this work by considering realistic outflow boundary conditions (Windkessel model). This complexity is addressed with the lifting function method, tipically used for the velocity, but introduced here also for the pressure. The method is validated both in a test case and in a patient-specific application.

Keywords: Cardiovascular flow, reduced order model, Galerkin projection, lifting function

1 Introduction

Heart disease represents one of the leading cause of death in the world, therefore several research areas pay particular consideration to cardiovascular disorders. In order to study the blood perfusion and the impact of some parameters on the blood flow in some relevant zones, mathematical models are built for patient-specific cases [1, 2, 3] or dedicated benchmarks [4]. In particular, a ROM is developed to obtain fast prediction by introducing at reduced level time dependent boundary conditions both for pressure and velocity.

2 Extended abstract content

The full order model describing the dynamics of the blood is composed by parametrized incompressible Navies-Stokes equations discretized by using the finite volume method. Time dependent boundary conditions are imposed on the inlet for the velocity and on the outlet for the pressure (Windkessel model).
Due to the large number of degrees of freedom involved for haemodynamics applications, a ROM is employed to speed up high fidelity simulations. A complete decoupling between two phases (offline and online) is one of the cornerstones of an efficient ROM framework. The main assumption is the possibility to write the reduced solution as the combination of a basis, which depends on space, and coefficients, associated only with time and/or parameters. During the offline phase, the full order solutions are computed over the cardiac cycle for different parameter values and the reduced basis space is extracted with the proper orthogonal decomposition algorithm. A Galerkin projection is performed to find a system for the reduced coefficients and the lifting function method is adopted to introduce non-homogeneous Dirichlet boundary conditions for the velocity field at reduced level. This approach is extended also for the outflow pressure [5]. Then, during the online stage the reduced system can be solved for every parameter value and the coefficients, combined with the basis, give efficiently the reduced solution.

3 Conclusions

The method is tested on an idealized benchmark, easy to handle, and on a patient specific case. The efficiency and the accuracy of the ROM framework are investigated with many comparisons and results.

References

[1] Balzotti C., Siena P., Girfoglio M., Quaini A., Rozza G. A data-driven reduced order method for parametric optimal blood flow control: Application to coronary bypass graft. Communications in Optimization Theory 2022; 26:1-19.

[2] Siena P., Girfoglio M., Ballarin F., Rozza G. Data-Driven Reduced Order Modelling for Patient-Specific Hemodynamics of Coronary Artery Bypass Grafts with Physical and Geometrical Parameters. Journal of Scientific Computing 2023; 94:38.

[3] Dueñas-Pamplona J., García J. G., Castro F., Muñoz-Paniagua J., Goicolea J., Sierra-Pallares J. Morphing the left atrium geometry: A deeper insight into blood stasis within the left atrial appendage. Applied Mathematical Modelling 2022; 108:27-45.

[4] Girfoglio M., Quaini A., Rozza G. A POD-Galerkin reduced order model for a LES filtering approach. Journal of Computational Physics 2021; 436:110260.

[5] Burkardt J., Gunzburger M., Lee H. C. POD and CVT-based reduced-order modeling of Navier–Stokes flows. Computer Methods in Applied Mechanics and Engineering 2006; 196(1-3):337-355.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A data-driven reduced-order model for real-time predictions applied to cardiovascular disease

Caterina Balzotti*, Pierfrancesco Siena*, Michele Girfoglio* and Gianluigi Rozza*

* SISSA International School for Advanced Studies
Mathematics Area, mathLab
Trieste, Italy
e-mail: cbalzott@sissa.it, psiena@sissa.it, mgirfogl@sissa.it, grozza@sissa.it

Abstract: Heart disease is one of the main cause of death worldwide and includes all diseases affecting the heart and/or blood vessels, such as coronary artery disease, arrhythmias and congenital heart defects. The study of mathematical models for the hemodynamics of blood flow in real time is attracting increasing interest from researchers. Our work aims at building a data-driven reduced order model (ROM) to simulate the hemodynamics of blood flow in real time, using a patient-specific geometry. The ROM relies on the proper orthogonal decomposition and supervised machine learning regression techniques. A careful analysis of the model's accuracy and computational cost is reported.

Keywords: Cardiovascular disease, reduced order models, data-driven, Navier-Stokes equations

1 Introduction

The goal of our work is the study of a data-driven reduced order model (ROM) to simulate blood flow dynamics in real time. The use of ROMs [1] to model cardiovascular disease is quite diffuse by now [2, 3, 4, 5], since it provides fast and accurate simulations of hemodynamics.

2 Extended abstract content

Let us consider a set $\mathcal{P}$ of parameters representing some physical conditions. To model blood flow dynamics we consider parametrized incompressible Navier-Stokes equations, whose numerical simulations are known to be very demanding from a computational point of view. Hereafter, we refer to the equations describing the problem as full order model (FOM). To reduce the computational cost of the numerical simulations we use the ROMs, which are usually divided into the offline and online phases. The offline phase consists in the collection of high fidelity solutions obtained by solving the FOM for a set of parameters $\mathcal{M} \subset \mathcal{P}$. These solutions are gathered into a matrix, from which the reduced basis space is extracted through the proper orthogonal decomposition algorithm. Finally, we use regression techniques to estimate the modal coefficients so that the approximated solution can be written as a linear combination between these coefficients and the reduced basis space. The regression technique used to estimate the modal coefficients is chosen to maximize the accuracy of the prediction. Although the offline phase could be expensive, it must be computed only once, while the online phase is reduced to a linear combination, thus it is naturally very fast.

3 Conclusions

We propose a data-driven ROM to simulate blood flow dynamics. The high computational times required by the FOM are highly reduced through the ROM, which at the same time is able to provide a reliable solution without a significant loss of accuracy.

References

[1] Hesthaven JS, Rozza G, Stamm B. Certified reduced basis methods for parametrized partial differential equations. Berlin: Springer; 2016.

[2] Ballarin F, Faggiano E, Ippolito S, Manzoni A, Quarteroni A, Rozza G, Scrofani R. Fast simulations of patient-specific haemodynamics of coronary artery bypass grafts based on a POD-Galerkin method and a vascular shape parametrization. J Comput Phys 2016; 315:609–628.

[3] Balzotti C, Siena P, Girfoglio M, Quaini A, Rozza G. A data-driven reduced order method for parametric optimal blood flow control: Application to coronary bypass graft. Commun. Optim. Theory 2022; 26:1–19.

[4] Buoso S, Manzoni A, Alkadhi H, Plass A, Quarteroni A, Kurtcuoglu V. Reduced-order modeling of blood flow for noninvasive functional evaluation of coronary artery disease. Biomech Model Mechanobiol 2019; 18(6):1867–1881.

[5] Siena P, Girfoglio M, Ballarin F, Rozza G. Data-Driven Reduced Order Modelling for Patient-Specific Hemodynamics of Coronary Artery Bypass Grafts with Physical and Geometrical Parameters. J Sci Comput 2023; 94:38.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modeling and Simulation of Prothrombin Activation Pathways in Pathological Blood Coagulation

Tobias Bongartz[*], Alessia Piergentili[†], Giulia Rossetti[†] and Marek Behr[*]

[*] Chair for Computational Analysis of Technical Systems
RWTH Aachen University
Aachen, Germany
{bongartz,behr}@cats.rwth-aachen.de

[†] Computational Biomedicine (IAS-5 / INM-9)
Forschungszentrum Jülich
Jülich, Germany
{a.piergentili,g.rossetti}@fz-juelich.de

Abstract: In this work, we present a mathematical model that predicts localized thrombus formation by taking into account the impact of changes in the prothrombin open/close ratio on blood clotting upon prothrombin mutations and ligand binding. This aspect is currently not considered by available mathematical models in the literature. The model is based on a set of convection-diffusion-reaction (CDR) equations that are coupled to the incompressible Navier-Stokes equations. Endothelial injuries/dysfunctions are modeled with boundary conditions to these equations, and the model is solved using a stabilized space-time finite element method. We apply this model to test cases with realistic blood-flow conditions and vessel geometries to investigate the impact of the prothrombin open/close ratio on thrombus formation and the potential for this ratio to be associated with pathologies.

Keywords: Thrombosis, Blood Coagulation, Prothrombin, Convection-Diffusion-Reaction Equations, Finite Elements

1. Prothrombin: Key Determinant in Blood Clotting

Vascular injury triggers an intrinsic biochemical response that prevents blood loss, however, excessive thrombosis can impede blood flow to vital organs and tissues [1]. Prothrombin, a pivotal component in the coagulation mechanism, is activated to thrombin, which subsequently catalyzes the activation of platelets, fibrin production and the amplification of the coagulation cascade. Recent studies [2] have shown that prothrombin exists in equilibrium between two forms: "closed" (~80%) and "open" (~20%). The binding of prothrombin to prothrombinase primarily occurs in the closed form, resulting in a more efficient conversion to thrombin. Thus, the ratio between the two forms of prothrombin is a crucial determinant of blood clotting and an imbalanced ratio may be associated with pathological conditions.

2. Advancing Thrombus Prediction Models

In this study, we present a mathematical model for the prediction of localized thrombus formation, incorporating key processes of human blood coagulation and analyzing the impact of various biological species. Specifically, we examine the incorporation of the prothrombin open/close ratio on blood coagulation in prothrombin mutations, including

potential benefits and uncertainties. This approach has not been previously considered in existing mathematical models in the literature [3].

3. Mathematical Modeling of Local Thrombus Formation

A mathematical model is presented that combines the incompressible Navier-Stokes equations convection-diffusion-reaction (CDR) equations. The model accounts for the impact of endothelial injuries and failures by incorporating appropriate boundary conditions. The solution is obtained using a stabilized space-time finite element method [4], and is applied to test cases that are representative of realistic blood flow conditions and vessel geometries.

References

[1] Spronk, H., Govers-Riemslag, J., & ten Cate, H. (2004). The blood coagulation system as a molecular machine. *BioEssays : News and Reviews in Molecular, Cellular and Developmental Biology, 25*, 1220–1228.

[2] Chinnaraj, M., Chen, Z., Pelc, L., Grese, Z., Bystranowska, D., Cera, E., & Pozzi, N. (2018). Structure of prothrombin in the closed form reveals new details on the mechanism of activation. *Scientific Reports,* 8.

[3] Zheng. (2020). A three-dimensional phase-field model for multiscale modeling of thrombus biomechanics in blood vessels. *PLOS Computational Biology*, 16(4), 1–24.

[4] Pauli, L., & Behr, M. (2017). On Stabilized Space-Time FEM for Anisotropic Meshes: Incompressible Navier-Stokes Equations and Applications to Blood Flow in Medical Devices. *International Journal for Numerical Methods in Fluids*, 85.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Strain-Based Blood Damage Modeling in Eulerian Frame

Nico Dirkes[1,*] **and Marek Behr**[1]

[1] Chair for Computational Analysis of Technical Systems
Center for Simulation and Data Science (JARA-CSD)
RWTH Aachen University
Schinkelstr. 2, 52062 Aachen, Germany
E-mail: {dirkes, behr}@cats.rwth-aachen.de

[*] Presenting author

Abstract: We present a method to quantify flow-induced red blood cell damage (hemolysis) in blood-handling medical devices. It is based on a Lagrangian model for red blood cell deformation. Using eigenvector decomposition, the Lagrangian formulation is transformed to an Eulerian description, enabling direct evaluation of the solution across the whole domain. The resulting model can be applied to any converged CFD simulation due to one-way coupling with the fluid velocity field. We compare the model to related blood damage models, highlighting their advantages and disadvantages. In particular, it is compared to a simplified Eulerian strain-based hemolysis model. The present model is shown to more accurately capture the behavior of the original Lagrangian cell deformation model, while the simplified model may yield inaccurate predictions for some flows. In this context, we discuss the applicability of these simplifications. We find that the new model combines the advantages of the simplified Eulerian model and the full Lagrangian model.

Keywords: Hemolysis, Blood damage, Ventricular Assist Devices, VAD, CFD, Biomedical engineering

1 Introduction

The design of blood-handling medical devices requires analysis of their biocompatibility. For this purpose, a model is applied to the flow field to estimate red blood cell damage (hemolysis) induced by fluid stress. Primitive blood damage models are based on a direct correlation of representative fluid stress to experimental hemolysis data [1]. More advanced models explicitly resolve red blood cell deformation in a Lagrangian description, e.g., by means of a morphology tensor [2]. The downside of this approach is that it requires pathline tracking, which complicates evaluation in critical regions such as boundary layers and recirculation zones, so an Eulerian description would be preferable. The aim of our work is to transform a Lagrangian strain-based model into Eulerian frame.

2 Proposed Model

The Lagrangian cell deformation model derived by Arora et al. [2] represents red blood cells as ellipsoids. Mathematically, they are described using a morphology tensor S, whose eigenvectors e_i represent the orientation of the ellipsoid's semi-axes and eigenvalues λ_i the respective lengths. The evolution equation for this morphology tensor was written as:

$$\frac{\mathrm{d}S}{\mathrm{d}t} - [\Omega,\, S] = -f_1\left(S - g\left(S\right) I\right) + f_2\left(ES + SE\right) + f_3\left[W - \Omega,\, S\right] . \tag{1}$$

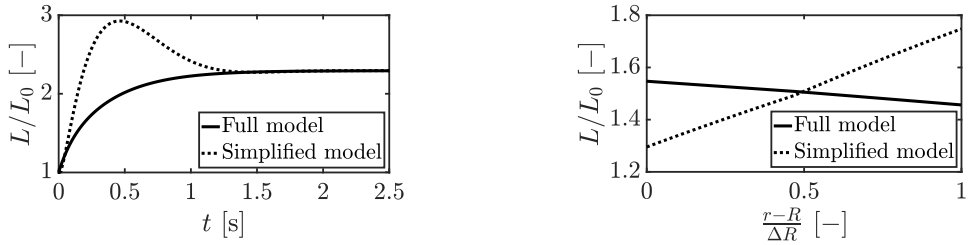


Figure 1: Cell deformation for plane (left) and counter-rotating circular (right) Couette flow

To obtain an Eulerian description, an eigenvector decomposition $Q^{\mathbf{T}}SQ = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ is carried out, yielding explicit transport equations for the eigenvalues and eigenvectors:

$$\frac{\partial \lambda_i}{\partial t} + (\mathbf{u} \cdot \boldsymbol{\nabla})\lambda_i = -f_1 \left(\lambda_i - \frac{3\lambda_1\lambda_2\lambda_3}{\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3} \right) + 2f_2\lambda_i\tilde{E}_{ii}\,, \tag{2}$$

$$\frac{\partial Q}{\partial t} + (\mathbf{u} \cdot \nabla)Q = Q\tilde{\Omega}\,, \qquad \tilde{\Omega}_{ij} = \frac{f_2}{f_3}\tilde{E}_{ij}\frac{\lambda_j + \lambda_i}{\lambda_j - \lambda_i} + \tilde{W}^*_{ij}\,, \qquad \tilde{E} = Q^{\mathbf{T}}EQ\,, \qquad \tilde{W}^* = Q^{\mathbf{T}}WQ\,. \tag{3}$$

This formulation is analytically equivalent to the original model (1). In contrast, the Eulerian formulation previously used by Pauli et al. [3] is obtained from eq. (1) by setting $\Omega = 0$. Figure 1 compares this simplified model to the full model. Starting from an arbitrary initial state in Couette flow, the simplified model predicts larger intermediate deformations before reaching a steady state, as the cell takes longer to align with respect to the plane of shear. Similar discrepancies are observed for rotating flow. Hence, the simplifications are only justified for flows that involve slow realignment of cells.

3 Conclusion

A strain-based blood damage model in an Eulerian frame was derived. Compared to previous Eulerian formulations, it yields more accurate hematological predictions. Compared to Lagrangian formulations, it can be evaluated on the whole domain more directly.

4 Acknowledgements

This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through grant 333849990/GRK2379 (IRTG Modern Inverse Problems).

References

[1] Giersiepen M, Wurzinger LJ, Opitz R, Reul H. Estimation of Shear Stress-related Blood Damage in Heart Valve Prostheses - in Vitro Comparison of 25 Aortic Valves. Int J Artif Organs 1990;13:300-306.

[2] Arora D, Behr M, Pasquali M. A tensor-based measure for estimating blood damage. Artif Organs 2004;28:1002-1015.

[3] Pauli L, Nam J, Pasquali M, Behr M. Transient stress-based and strain-based hemolysis estimation in a simplified blood pump. Int J Numer Method Biomed Eng 2013;29:1148-1160.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Anisotropic electrical conductivity of blood: a new model for numerical computations of impedance cardiography signals

Alireza jafarinia*, Vahid Badeli† Gian Marco Melito ‡,Alice Reinbacher-Köstinger†, Günter Brenn§, Mandfred Kaltenbacher†, Thomas Hochrainer*

* Institute of Strength of Materials
Graz University of Technology
Graz, Austria
e-mail: alireza.jafarinia@tugraz.at, hochrainer@tugraz.at

† Institute of Fundamentals and Theory in Electrical Engineering
Graz University of Technology
Graz, Austria
e-mail: vahid.badeli@tugraz.at, manfred.kaltenbacher@tugraz.at, alice.koestinger@tugraz.at

‡ Institute of Mechanics
Graz University of Technology
Graz, Austria
e-mail: gmelito@tugraz.at

§ Institute of Fluid Mechanics and Heat Transfer
Graz University of Technology
Graz, Austria
e-mail: guenter.brenn@tugraz.at

Abstract: Impedance cardiography (ICG) is a non-invasive and low-cost method in which the impedance is measured by injecting a low-magnitude electrical current into the surface of the thorax. The impedance changes during cardiac cycles mainly depend on the blood's electrical conductivity and volume changes. The blood conductivity depends on hemodynamic conditions [1]. Therefore, ICG may be beneficial for diagnosing and monitoring cardiovascular diseases where the hemodynamic conditions are compromised [1, 2]. Numerically calculated ICG signals may facilitate establishing ICG for detecting and monitoring cardiovascular diseases. However, a three-dimensional model of the anisotropic and dynamically changing conductivity of blood is as yet not available. The source of the anisotropic electrical conductivity in the blood flow is the orientation of the oblate and biconcavely shaped red blood cells (RBCs) [2, 3], which may be treated as non-conductive particles up to electrical frequencies of 1 MHz [4].

In the current study, a new model for computing the anisotropic electrical conductivity of blood is developed. The new model is based on the experimental observation of RBC motions in shear flows [5, 6], and the two-dimensional conductivity model proposed by Gaw et al. [3]. The new three-dimensional model allows for computing the blood conductivity at any point in the blood flow field based on the fluid velocity and the extra stress tensor.

The new model is incorporated into computational fluid dynamics (CFD) simulations of blood flow in a straight vessel and in an idealized aorta to examine the model's applicability. The results are in qualitative agreement with the studies of Gaw et al. [3], where the blood conductivity in the flow direction for a straight vessel was computed. Although all the results are in qualitative agreement with available literature studies, validation of the model with

experiments is yet outstanding. For validation, experiments will be performed to measure the blood flow-related impedance changes in different geometries.

Keywords: Blood electrical conductivity, Anisotropic conductivity, Impedance cardiography, Cardiovascular diseases

Acknowledgements: This work was funded by Graz University of Technology, Austria, through the LEAD Project on Mechanics, Modeling, and Simulation of Aortic Dissection.

References

[1] Badeli V, Melito GM, Reinbacher-Köstinger A, Biro O, Ellermann K. Electrode positioning to investigate the changes of the thoracic bioimpedance caused by aortic dissection–a simulation study. JoEB 2020;11:38-48.

[2] Badeli V, Jafarinia A, Melito GM, Müller TS,Reinbacher-Köstinger A, Hochrainer T, Brenn, G, Ellermann K, Biro O, Kaltenbacher M. Monitoring of false lumen thrombosis in type B aortic dissection by impedance cardiography–A multiphysics simulation study. Int. J. Numer. Method Biomed. Eng. 2022;e3669.

[3] Gaw RL, Cornish BH, Thomas BJ. The electrical impedance of pulsatile blood flowing through rigid tubes: a theoretical investigation. IEEE. Trans. Biomed. Eng. 2008;55:721-727.

[4] Hoetink AE, Faes TJC, Visser KR, Heethaar RM. On the flow dependency of the electrical conductivity of blood. IEEE. Trans. Biomed. Eng. 2004;21:1251-1261.

[5] Fischer TM, Stöhr-Liesen M, Schmid-Schönbein H. The Red Cell as a Fluid Droplet: Tank Tread-Like Motion of the Human Erythrocyte Membrane in Shear Flow. AAAS 1978;202:894-896.

[6] Goldsmith HL, Marlow J, MacIntosh FC. Flow behaviour of erythrocytes-I. Rotation and deformation in dilute suspensions. Proc. R. Soc. Lond. B Biol. Sci. 1972;182:351-384.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Quantitative assessment of the variability of FFR_{CT} due to minimal uncertainty in lumen segmentation threshold

Daniel Fernández-Martínez[*†], Jose M. Montanero[†], María Reyes González-Fernández[††], Juan Manuel Nogales-Asensio[††] and Conrado Ferrera[†]

[†] Departmento de Ingeniería Mecánica, Energética y de los Materiales
Escuela de Ingenierías Industriales, Universidad de Extremadura
Badajoz, Spain
[*]e-mail: danielfm@unex.es

[††] Sección de Hemodinámica y Cardiología Intervencionista, Servicio de Cardiología
Hospital Universitario de Badajoz
Badajoz, Spain

Abstract: Computational Fractional Flow Reserve (FFR_{CT}) is increasingly used for non-invasive diagnosis of cardiovascular disease in coronary arteries in order to guide revascularization decisions. Quantitative assessment of the variability of FFR_{CT} due to input uncertainty is a key step towards its integration into a clinical setting, especially when FFR is in the gray zone $[0.75 - 0.8]$. When this value falls below this range, myocardial ishemia is highly possible. These types of simulations require accurate 3D reconstruction of the coronary bed and tuning patient-specific lumped parameter models. There are some works that have investigated different geometric and input uncertainties in patient-specific coronary simulations. However, it is not clear whether minimal perturbations in the global lumen segmentation threshold decrease the estimate of FFR_{CT}. In this preliminary work, we address this issue. The average variation observed is about four times less compared with the obtained through the repetition of invasive catheterization. Thus, we prove that FFR_{CT} is a reliable and robust procedure in terms of minimal global lumen segmentation uncertainty.

Keywords: FFR_{CT}, computational fluid dynamics, coronary arteries modeling, lumen segmentation uncertainty

1 Introduction

In recent years, in-silico simulations combining Coronary Computed Tomography Angiography (CCTA) with Computational Fluid Dynamics (CFD) have been proposed as a non-invasive alternative for the evaluation of stenosis severity in coronaries [1]. However, it is crucial to investigate the robustness of this method against input uncertainties. Although some works have addressed this issue [2, 3], uncertainty in the lumen diameter due to limitations in the resolution image or intra-observer variability remains unclear. To fill this gap, we have performed a computational study to explore if minimal perturbations during the segmentation procedure are enough to get a mismatch in the computation of the FFR_{CT}.

2 Materials and methods

Figure 1 summarizes the general workflow of this study. Several anonymous patients with moderate coronary lesions (FFR near the 0.8 cutoff) were selected. CCTA images were

collected and segmented in order to reconstruct the coronary tree and the left ventricle (LV), based on an optimal global lumen segmentation threshold. Minimal threshold perturbations ($\pm 10HU$) were made to obtain 2 variations of each patient's anatomy. Patient-specific open-loop OD coronary lumped parameter networks combined with allometric scaling laws were tuned and coupled to the 3D simulation to mimic the pulsatile and diastolic-predominant flow present in coronary arteries. Simulations of the optimal segmented fluid domain, as well as its variants, were performed until the results match the obtained by the Invasive Coronary Angiography (ICA).

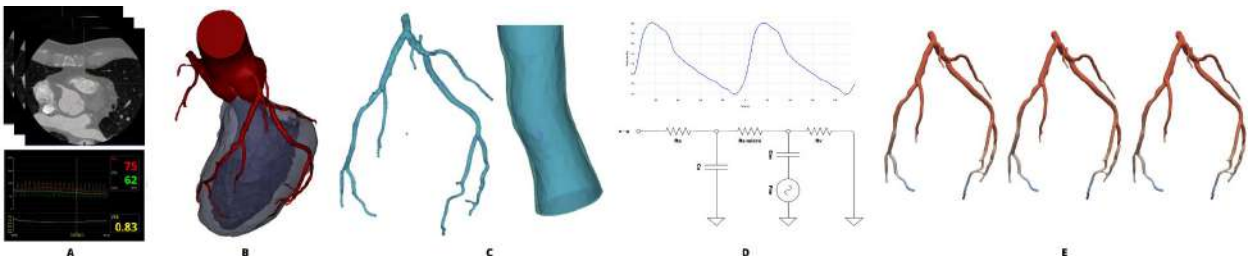


Figure 1: **A**: CCTA segmentation and ICA. **B**: Coronary tree and LV 3D reconstruction. **C**: Threshold-based variations. **D**: Patient-specific inlet and outlet boundary conditions. **E**: Pressure / FFR_{CT} contours.

3 Results and conclusions

We present a computational study confirming that intra-observer variations in the global lumen segmentation threshold do not imply a relevant mismatch in FFR_{CT} in patients with moderate coronary lessions. The average variation observed is about four times less compared with the obtained through the repetition of the invasive catheterization [2]. Further research is needed to extrapolate the results to mild and severe vessel stenosis, although accurate segmentation in these cases is not so critical since FFR is not close to the cutoff.

4 Acknowledgements

This work was supported by Junta de Extremadura under the **IB20105** contract (partially financed by FEDER).

References

[1] Taylor CA, Fonte TA, Min JK. Computational fluid dynamics applied to cardiac computed tomography for noninvasive quantification of fractional flow reserve: scientific basis. J Am Coll Cardiol. 2013 Jun 4;61(22):2233-41

[2] Sankaran S, Kim HJ, Choi G, Taylor CA. Uncertainty quantification in coronary blood flow simulations: Impact of geometry, boundary conditions and blood viscosity. J Biomech. 2016 Aug 16;49(12):2540-7.

[3] Seo, J, Schiavazzi, DE, Kahn, AM, Marsden, AL. The effects of clinically-derived parametric data uncertainty in patient-specific coronary simulations with deformable walls. Int J Numer Meth Biomed Engng. 2020; 36:e3351.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Consistent fractional-step methods for incompressible viscoelastic flows

Pacheco, Douglas R. Q. – Norwegian University of Science and Technology, Trondheim, Norway, e-mail: douglas.r.q.pacheco@ntnu.no

Castillo, Ernesto – University of Santiago de Chile, Santiago, Chile, e-mail: ernesto.castillode@usach.cl

Abstract: Simulating viscoelastic fluid flows is a highly challenging task that demands robust and efficient numerical solvers. The viscoelastic equations form a mixed problem combining the Navier–Stokes system with a dynamic, tensor-valued equation, which increases mathematical and computational demands. Hence, methods decoupling the calculation of the flow quantities are particularly attractive. In consistent fractional-step schemes, the equations are split from the continuous level, so that neither mass nor momentum balance are, a priori, violated. Therefore, there is no need for corrections or velocity projections, which results in fewer steps than other standard approaches. Furthermore, consistency eliminates both numerical boundary layers and splitting errors, which enables high-order accuracy in space and time. In this talk, we present new consistent splitting methods for incompressible viscoelastic flows, with arbitrary constitutive laws allowed. We present the method and its algorithm, along with numerical examples. Both optimal convergence and good numerical stability are verified through challenging benchmark problems.

Keywords: Viscoelastic fluids, Fractional-step methods, High-order methods, Finite element method.

1. Introduction

Herein, we shall use *splitting schemes* and *fractional-step methods* as interchangeable terms. For an overview of the state of the art on splitting methods for viscoelastic flow problems, the reader is referred to our recent article [1] and the references therein.

The Navier–Stokes momentum equation for an incompressible, isothermal, viscoelastic fluid flow can be written as

$$\frac{\partial u}{\partial t} + (\nabla u)u - \beta\nu_0\Delta u - \nabla\cdot\sigma + \nabla p = g\,, \tag{1}$$

where (u, p, σ) are the velocity, pressure and extra stress fields, g is a forcing term and $\beta \in [0,1]$ is a dimensionless parameter defining the amount of solvent viscosity $\beta\nu_0$ and polymeric viscosity $(1-\beta)\nu_0$. In addition, we have the incompressibility constraint,

$$\nabla\cdot u = 0\,, \tag{2}$$

and a dynamic equation for the extra stress tensor σ, which depends on the viscoelastic model adopted. For simplicity, we consider the Oldroyd-B model, which in Einstein notation reads

$$\frac{\partial\sigma_{ij}}{\partial t} + \frac{\sigma_{ij}}{\lambda} + u\cdot\nabla\sigma_{ij} = \frac{(1-\beta)\nu_0}{\lambda}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \sigma_{kj}\frac{\partial u_i}{\partial x_k} + \sigma_{ik}\frac{\partial u_j}{\partial x_k}\,. \tag{3}$$

The model is then closed with initial and boundary conditions for the momentum equation, plus initial stress conditions (a stress equation such as (3) requires no boundary conditions).

2. Splitting framework

The first family of *consistent* splitting methods for incompressible flow problems was conceived by Johnston and Liu [2]. The key idea behind such schemes is to derive, at the fully continuous level (and *not* at the semi-discrete one, as projection methods do), a pressure equation that can replace the divergence-free constraint (2). Moreover, this equation and its boundary conditions must be consistent – albeit artificial – with the solution of the continuous problem. For the viscoelastic case, we can replace explicit incompressibility by the Poisson equation

$$-\Delta p = \nabla \cdot [\beta \nu_0 \nabla \times (\nabla \times u) + (\nabla u)u - \nabla \cdot \sigma - g] - \alpha \nabla \cdot u\,, \tag{4}$$

together with boundary conditions that depend on what kind of Cauchy data is being considered for the momentum equation (1). While it is quite straightforward to verify that this equation is satisfied by the solution (u, p, σ) of Eqs. (1)-(3), proving that it implies Eq. (2) is more involved, so the reader is referred to our recent article [1]. The factor α in Eq. (4) is a non-negative user-defined parameter [1,2]. Most importantly, Eq. (4) can *consistently* replace the continuity equation (2) regardless of which viscoelastic model is used for σ.

By replacing Eq. (2) with Eq. (4), we end up with an equation to find the pressure p, given u and σ. Therefore, in a time-dependent problem, we can first solve the velocity-stress system using an extrapolated pressure, and then use the updated values of (u, σ) to find the new pressure. Although one can solve for velocity and stress in a monolithic fashion, it is *especially* advantageous to decouple the computation of those unknowns, as that reduces the overhead due to the additional (tensor-valued) unknown σ in a viscoelastic system. The idea is to use a backward differentiation formula (BDF) on both the momentum and stress equations, and leverage extrapolation of selected terms to decouple not only u from σ, but also the individual *components* of each unknown.

For the momentum step, this corresponds to writing, at time $t = t_{n+1}$, the linearised equation

$$\delta_t u_{n+1} + (\nabla u_{n+1})u^* - \beta \nu_0 \Delta u_{n+1} - \nabla \cdot \sigma^* + \nabla p^* = g_{n+1}\,, \tag{4}$$

where δ_t and the superscripted asterisk $(*)$ denote, respectively, the finite difference and extrapolation operators of matching order. After solving Eq. (4) for u_{n+1}, component-wise, we can use the updated velocity in the stress equation. Notice that semi-discrete schemes can also be used in Eq. (3) to decouple the computation of the stress components [3].

3. Conclusions

The purpose of this extended abstract was to present the key ideas behind consistent splitting methods for viscoelastic flows. While discussing discretisation details is out of the scope of the abstract *per se*, in the conference talk we shall present several possibilities, considering BDFs of different order in time, various finite element combinations in space, together with numerical results demonstrating the efficiency and accuracy of our splitting framework.

Acknowledgements

The second author acknowledges the support given by the Agencia Nacional de Investigación y Desarrollo (ANID) through the project FONDECYT 1210156.

References

[1] Pacheco DRQ and Castillo E. Consistent splitting schemes for incompressible viscoelastic flow problems. Int. J. Numer. Methods. Eng. 2023; 124(8):1908-1927.

[2] Johnston H and Liu JG. Accurate, stable and efficient Navier–Stokes solvers based on explicit treatment of the pressure term. J. Comput. Phys. 2004;199(1):221-259.

[3] Ravindran SS. Analysis of a second-order decoupled time-stepping scheme for transient viscoelastic flows. Int. J. Numer. Anal. Model. 2020;17(1):87-109.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Multiphysical simulation of flow-related impedance changes in arteries

Vahid Badeli[†], Alireza Jafarinia[*], Alice Reinbacher-Köstinger[†], Thomas Hochrainer[*], Mandfred Kaltenbacher[†]

[†] Institute of Fundamentals and Theory in Electrical Engineering
Graz University of Technology
Graz, Austria
e-mail: vahid.badeli@tugraz.at, alice.koestinger@tugraz.at, manfred.kaltenbacher@tugraz.at

[*] Institute of Strength of Materials
Graz University of Technology
Graz, Austria
e-mail: alireza.jafarinia@tugraz.at, hochrainer@tugraz.at

Abstract: Bioimpedance methods, such as impedance cardiography (ICG) and impedance plethysmography (IPG), provide a non-invasive, time-continuous, cheap, and convenient technology for determining cardiodynamic parameters. A lack of and difficult accessibility to data obstructed the improvement of signal interpretability and parameter estimation accuracy hence widespread clinical adoption [1]. The limitations mentioned above need to be overcome with multi-physics simulations of different scenarios.

In IPG and ICG, a low-magnitude, low-frequency electrical current is injected by two electrodes into the body segment. Then, the voltage is measured via two pick-up electrodes located between the injection electrodes. Since blood's electrical conductivity is much higher than other tissues in the measurement region, the impedance changes mainly originate from the blood volume changes in the artery during systolic and diastolic phases, and the velocity-induced electrical conductivity changes [2]. Therefore, ICG and IPG have been suggested for diagnosing arterial diseases such as occlusion, stenosis, dissection, and thrombosis, which affect the blood flow in the arteries significantly [2, 3].

The electrical conductivity of flowing blood is anisotropic and depends on the hemodynamic conditions. Therefore, in this work, a computational fluid dynamic simulation (CFD) has been set up in OpenFOAM software [4] to model the blood flow in the arteries from which the anisotropic electrical conductivity of blood is computed as a time-dependent tensor field using a novel method presented in [5]. Furthermore, a 3D FEM electric simulation model has been set up in OpenCFS software [6] based on a simplified geometry of the body segment to solve the time-harmonic current flow problem. By injecting an alternating current with a magnitude of $|\underline{I_0}|$ and a frequency of f into the source electrodes, the electric potential V can be calculated by solving the Laplace equation

$$\nabla \cdot [(\sigma + \mathrm{j}\omega\varepsilon)\, \nabla V] = 0\,, \tag{1}$$

and considering suitable boundary conditions. In (1), ω, σ, and ε are the angular frequency, the electric conductivity, and the electric permittivity, respectively. All tissue types' electric conductivity and permittivity are taken from the literature [7]. In order to consider the blood flow-induced conductivity changes during the cardiac phases, we use the conductivity

tensor field obtained from CFD simulations. For this purpose, the blood conductivity data has been interpolated from the volume grid in the CFD model to the FEM grid in the electric simulation model. Finally, the voltage drop and impedance between two pick-up electrodes can be evaluated for each simulation time step.

The results obtained from simulating different arteries, i.e., flow-related impedance curves, show the developed framework's capability to investigate the impact of different pathologies on the bioimpedance signals. The clinical verification for specific diseases is currently in progress, which will allow model verification by patient-specific studies.

Keywords: Blood electrical conductivity, Multiphysics simulation, Bioimpedance, Arterial diseases

1 Acknowledgements

This work is funded by Graz University of Technology, Austria, through the LEAD Project on Mechanics, Modeling, and Simulation of Aortic Dissection.

References

[1] Mansouri S, Alharbi Y, Alshrouf A, and Alghahtani A. Cardiovascular diseases diagnosis by impedance cardiography. J Electr Bioimp, vol. 13, pp. 88-95, 2022.

[2] Badeli V, Melito GM, Reinbacher-Köstinger A, Biro O, Ellermann K. Electrode positioning to investigate the changes of the thoracic bioimpedance caused by aortic dissection–a simulation study. J Electr Bioimp, vol. 11, pp. 38-48, 2020.

[3] Badeli V, Jafarinia A, Melito GM, Müller TS, Reinbacher-Köstinger A, Hochrainer T, Brenn, G, Ellermann K, Biro O, Kaltenbacher M. Monitoring of false lumen thrombosis in type B aortic dissection by impedance cardiography – A multiphysics simulation study. Int J Numer Meth Biomed Engng. 2022;e3669. doi:10.1002/cnm.3669

[4] http://www.openfoam.org.

[5] Jafarinia A, Badeli V, Melito GM, Reinbacher-Köstinger A, Brenn G, Kaltenbacher M, Hochrainer T. Anisotropic electrical conductivity of blood: a new model for numerical computations of impedance cardiography signals. VII ECCOMAS Young Investigators Conference YIC2023 19-21 June 2023, Porto, Portugal.

[6] https://opencfs.org.

[7] Gabriel S. The dielectric properties of biological tissues Physics in Medicine and Biology. 41:2231-2249, 1996.

A finite element approach to simulating columnar solidification for the prediction of macrosegregation in binary alloys

Richard W. Olley[1*], Ignatios Athanasiadis[1], Andrei G. Shvarts[1], Łukasz Kaczmarczyk[1], Chris J. Pearce[1]

[1] Glasgow Computational Engineering Centre, James Watt School of Engineering, University of Glasgow, Glasgow, UK.

Abstract

Macrosegregation is the compositional variation of an alloy in the order of cm and mm, which occurs during solidification. A finite element model is presented for the prediction of macrosegregation in binary alloys utilising a monolithic solution scheme. In this work, we present simulations of Pb-18wt% Sn and Sn-10wt% Pb binary alloys assuming columnar solidification with the Lever rule assumption at the microscopic scale. The simulation of the Pb-18wt% Sn alloy is in response to a call from [1], for benchmarking columnar solidification models in the macrosegregation modelling field. The model requires solving the conservation equations of: mass, momentum, energy and species. A monolithic scheme is therefore proposed, encompassing full coupling between these conservation equations. The Taylor-Hood element is chosen for solving Navier-Stokes equations, where both velocity and pressure fields are sought in the H1 energy space. Choosing this element, which is also known to theoretically exhibit an optimal convergence rate, allows for an arbitrary choice of approximation order, P, for the various approximated fields enabling exploitation of higher polynomial orders where necessary (p-refinement). Macrosegregation maps obtained during solidification show good agreement with other finite element columnar solidification models in literature [2, 3]. The proposed model has been developed as a module in the open-source finite element code MoFEM [4] envisaged to enhance on-site industrial procedures. This module architecture allows for an easily extendable and versatile implementation of multi-phase macrosegregation models alongside single-phase models.

Key words: *Macrosegregation modelling; Navier-Stokes; Taylor-Hood element; Solidification; Thermo-solutal buoyancy; Lever rule*

References

[1] Michel Bellet, H Combeau, Y Fautrelle, D Gobin, M Rady, E Arquis, O Budenkova, B Dussoubs, Y Duterrail, A Kumar, et al. Call for contributions to a numerical benchmark problem for 2d columnar solidification of binary alloys. *International Journal of Thermal Sciences*, 48(11):2013–2016, 2009.

[2] Qipeng Chen and Houfa Shen. A finite element method for prediction of macrosegregation with solidification columnar. *Journal of International Scientific Publications: Materials, Methods and Technologies (Online)*, 14:1–8, 2020.

[3] Hervé Combeau, Michel Bellet, Yves Fautrelle, Dominique Gobin, Eric Arquis, Olga Budenkova, Bernard Dussoubs, Yves Du Terrail, Arvind Kumar, Ch-A Gandin, et al. Analysis of a numerical benchmark for columnar solidification of binary alloys. In *IOP Conference Series: Materials Science and Engineering*, volume 33, page 012086. IOP Publishing, 2012.

[4] Łukasz Kaczmarczyk, Zahur Ullah, Karol Lewandowski, Xuan Meng, Xiao-Yi Zhou, Ignatios Athanasiadis, Hoang Nguyen, Christophe-Alexandre Chalons-Mouriesse, Euan J Richardson, Euan Miur, et al. Mofem: An open source, parallel finite element library. *Journal of Open Source Software*, 5(45):1441, 2020.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A finite element model updating approach for the characterisation of piezoelectric materials

Ignatios Athanasiadis[1*], Andrei Shvarts[1], Sakineh Fotouhi[2], Łukasz Kaczmarczyk[1], Sandy Cohran[2], Chris Pearce[1]

[1]Glasgow Computational Engineering Centre, James Watt School of Engineering, University of Glasgow
[*]e-mail: ignatios.athanasiadis@glasgow.ac.uk

[2]Centre of Medical and Industrial Ultrasonics, James Watt School of Engineering, University of Glasgow

Abstract: The physical response of piezoelectric materials is governed by the strong coupling of mechanical and electrical phenomena as their mechanical deformation generates electric potential gradients and vice versa. There has been an increasing interest in these materials due to the breadth of engineering applications where they have been successfully used, such as power harvesting and smart sensing [1, 2]. Therefore, the accurate determination of piezoelectric materials' parameters is essential which has lead to an increasing demand for improved numerical tools to support this scope. In this work, we propose a coupled numerical framework for piezoelectric material characterisation. For our analysis, experimentally obtained electric impedance phase diagrams are used, where a cubic specimen is subjected to a voltage pulse that generates its mechanical and voltage damping oscillation. Thereafter, the experimentally obtained resonance frequencies and their amplitude are used to determine a set of objective functions that are minimised via the Finite Element Model Updating method (FEMU) in order to find the material parameters. The minimisation procedure involves a series of fully implicit dynamic FEM analyses with changing the material input parameters between simulations. The FEM analyses are performed using the open source software MoFEM [3] and the optimisation algorithms used for the material parameter calibration are found in open source libraries in python. The framework is implemented in an automated manner as the two aforementioned computational tools and the associated pre-processing and post-processing are integrated in a cloud-based JupyterHub server and are accessed by a single Jupyter notebook. The proposed framework is aimed to be used to aid new piezoelectric material technologies where more complex structures are involved and to be extended to account for more physical phenomena.

Keywords: piezoelectric, hierarchical basis, dynamic analysis, material characterisation, optimisation

References

[1] S. Cochran. 1 - piezoelectricity and basic configurations for piezoelectric ultrasonic transducers. In Ultrasonic Transducers, Woodhead Publishing Series in Electronic and Optical Materials, pages 3–35. Woodhead Publishing, 2012.

[2] Susmriti Das Mahapatra, et al. Piezoelectric materials for energy harvesting and sensing applications: Roadmap for future smart materials. Advanced Science, 8(17):2100864, 2021.

[3] Lukasz Kaczmarczyk, et al. Mofem: An open source, parallel finite element library. Journal of Open Source Software, 5(45):1441, 2020

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A two-scale thermo-hydro-mechanical model for supra-glacial lake driven fracture through ice-sheets

Tim Hageman[*], **Ravindra Duddu**[†], **Emilio Martínez-Pañeda**[*]

[*] Department of Civil and Environmental Engineering
Imperial College London
London, UK
e-mail: t.hageman@imperial.ac.uk

[†] Department of Civil and Environmental Engineering
Vanderbilt University
Nashville, USA

Abstract: Drainage of supra-glacial lakes has a profound impact on glacial movements. However, due to the complexity of this process, it is often simulated through a vast set of assumptions. Here, we present a numerical two-scale approach to capture the relevant mechanics of the hydraulic fracturing process. The displacements of the ice-sheet are captured as a visco-elastic solid through finite elements, while the fluid contained within the crevasse is modelled as a one-dimensional discontinuity using interface elements. The fluid velocity and thermal processes (heat transfer, melting, and freezing) are solved as small-scale problem on a per-integration-point basis, which is then coupled to the large scale equations in a consistent manner. This two-scale approach contains all thermal processes to the small-scale, thus removing the need to solve thermal throughout the glacier. As a result, the described scheme is capable of simulating ice-sheet scale cases (with dimensions in the order of kilometres), while still capturing the processes occurring within crevasses with only a limited opening height (order of centimetre to metre), as is demonstrated through typical ice-sheet fracture cases.

Keywords: Ice-sheets, hydro-fracture, two-scale approach, interface elements, thermal

1 Introduction

Drainage of lakes located atop of ice-sheets has a strong impact on the overall movement of ice-sheets and glaciers: As crevasses develop, the lake water is transported from the surface to the bed, where it reduces the friction experienced by the ice and accelerates its movement towards and eventual collapse into the oceans [1]. As such, developing an in-depth understanding and being able to predict these processes is paramount to estimating the effects of climate change on sea-level rise [2]. However, models predicting these phenomena are often overly simplified or limited in scope, for instance solely modelling the uplifting processes but neglecting the actual fracture mechanics. The few models that do include fracture mechanics within their simulations often still neglect the effects of the fluid flow,

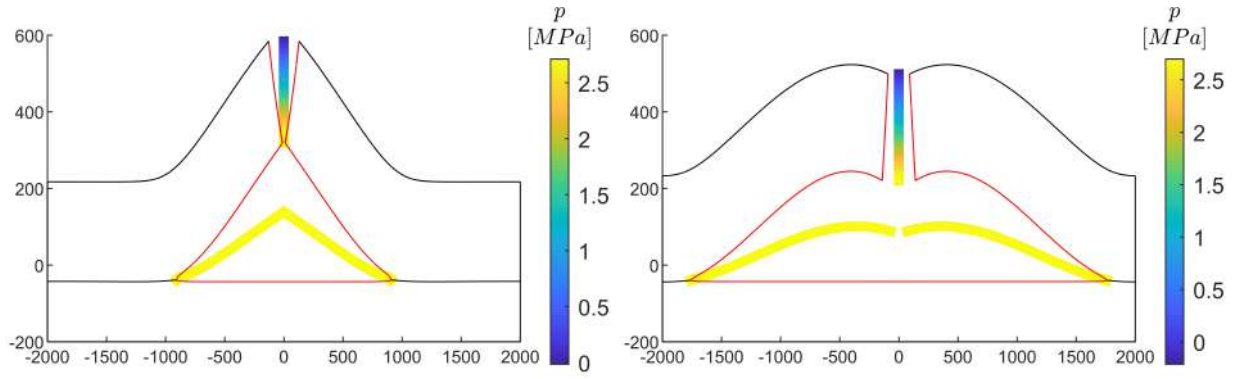


Figure 1: Deformations of the ice-sheet (magnified by a factor $\times 1000$) and fluid pressure within the crevasse after 1 hour using a visco-elastic (left) and linear-elastic (right) ice rheology.

electing to apply a pre-determined and static water level within the crevasses [4]. Even though the water-filled crevasse is in direct contact with sub-zero ice-sheets, these thermal processes are always neglected within numerical simulations.

2 Model overview

Here, we present a numerical model that does include these thermal effects and explicitly simulates the fluid flow through the crevasses. The deformations of the ice-sheet are captured through the momentum balance, assuming either a linear-elastic rheology of the ice-sheet, or a visco-elastic rheology using Glenn's law to ore accurately capture the long-term behaviour.

The fluid contained within the crevasse is approximated through a two-scale approach [5]: The mass balance for the water contained within the crevasse is averaged over the crevasse opening height, reducing the two-dimensional crevasse to a one-dimensional discontinuity line. The fluid fluxes required in this mass balance, together with the thermal balance are resolved as small-scale problem within each integration point, translating the large-scale pressure and displacements into unidirectional fluid fluxes while retaining the local heat fluxes and melting rates as history-dependent local variables.

The resulting equations are implemented in a finite element scheme, dynamically inserting new interface elements as the crevasse propagates. The small-scale problem is not only used within this scheme to obtain the fluid fluxes, but consistent tangential matrices are also extracted from the small-scale problem to assemble the global tangential stiffness matrix, allowing for a well-converging scheme.

3 Results

The resulting scheme is able to simulate hydraulic fracturing and the subsequent lake drainage, using both a linear-elastic and visco-elastic ice-sheet rheology, shown in Figure 1. Even though the viscous effects are commonly assumed to be negligible at these small time-scales, it is observed that due to the large hydraulic pressures involved the viscous creep has a significant effect on the drainage rates. Simulations for varying ice-sheet temperatures furthermore show a temperature "barrier" below which cracks freeze before the hydraulic fracture can reach the bed, while above this limit the crevasse is capable of draining complete lakes within hours.

References

[1] Siegert, M, Alley, RB, Rignot, E, Englander, J, Corell, R. Twenty-first century sea-level rise could exceed IPCC projections for strong-warming futures. One Earth 2020; 3(6), 691–703.

[2] Das, SB, Joughin, I, Behn, MD, Howat, IM, King, MA, Lizarralde, D, Bhatia, MP. Fracture propagation to the base of the Greenland ice sheet during supraglacial lake drainage. Science 2008; 320(5877), 778–781.

[3] Rice, JR, Tsai, VC, Fernandes, MC, Platt, JD. Time scale for rapid draining of a surficial lake into the Greenland ice sheet. J. Appl. Mech. 2015; 82(7).

[4] Clayton, T, Duddu, R, Siegert, M, Martínez-Pañeda, E. A stress-based poro-damage phase field model for hydrofracturing of creeping glaciers and ice shelves. Eng. Fract. Mech. 2022; 272, 108693.

[5] Hageman, T, Pervaiz Fathima, KM, de Borst, R. Isogeometric analysis of fracture propagation in saturated porous media due to a pressurised non-Newtonian fluid. Comp. Geotech. 2019; 112, 272–283.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Edge-preserving inversion with heavy-tailed Bayesian neural networks priors

Senchukova Angelina*, Uribe Felipe*, De Wiljes Jana† and Roininen Lassi*

* Department of Computational Engineering
School of Engineering Science (LENS), Lappeenranta–Lahti University of Technology LUT
Lappeenranta, Finland
e-mail: name.surname@lut.fi

† Institute for Mathematics, University of Potsdam
Potsdam-Golm, Germany
e-mail: wiljes@uni-potsdam.de

Abstract: We study Bayesian inverse problems where the unknown target function is piecewise constant. Priors based on neural networks with heavy-tailed-distributed weights/biases have been employed due to their discretization-independent property and ability to capture discontinuities. We aim at developing neural network priors whose parameters are drawn from Student's t distributions. The idea is to parameterize the unknown function using a neural network which sets a finite-dimensional inference framework. This requires finding the posterior distribution of the weights/biases of the network representation. The resulting posterior is, however, high-dimensional and multimodal which makes it difficult to characterize using traditional sampling algorithms. Therefore, we explore data assimilation techniques, such as particle and ensemble Kalman filters to sample the posterior distribution more effectively. As a numerical example, we consider a simple signal deconvolution to illustrate the properties of the prior.

Keywords: Bayesian Inverse Problems, Bayesian Neural Network Priors, Heavy-Tailed Priors

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Convergence rates of non-stationary and deep Gaussian process regression

Conor Osborne* **and Aretha Teckentrup†**

* Department of Mathematics
University of Edinburgh
Edinburgh, UK
e-mail: conor.osborne@ed.ac.uk

† Department of Mathematics
University of Edinburgh
Edinburgh, UK
e-mail: a.teckentrup@ed.ac.uk

Abstract: Gaussian processes have proved to be a powerful and flexible tool in the reconstruction of functions given a set of known training points, with applications in machine learning, optimisation and data assimilation. However, they can be limited when the functions being reconstructed are of a non-stationary or anisotropic nature. Deep Gaussian processes, constructed using a hierarchical process where the inputs to a Gaussian process are themselves Gaussian processes, aim to give a more flexible approach to function reconstruction. We look at convergence rates of these deep Gaussian processes in terms of the number of known training points. We also show that deep Gaussian process regression achieves considerably better results than standard Gaussian process regression when reconstructing non-stationary and anisotropic functions.

Keywords: Gaussian process regression, non-stationary Gaussian processes, deep Gaussian processes, convergence rates, Bayesian inverse problems, posterior contraction

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Reduced Kalman inversion in multiscale models via deep learning

Yankun Hong[*,†], **Harshit Bansal**[*] **and Karen Veroy**[*]

[*] Department of Mathematics and Computer Science
Eindhoven University of Technology
Eindhoven, The Netherlands
[†]e-mail: y.hong@tue.nl

Abstract: In the context of nonlinear multi-scale problems, estimating the macroscopic distribution of microscopic geometrical parameters given macroscopic measurements is of interest. In general, such inverse estimation is challenging due to *(i)* the need for derivatives of the complex multi-scale forward simulation, which requires a non-linear macro-scale and multiple non-linear micro-scale simulation(s), *(ii)* the typically high computational cost of the forward solver, and *(iii)* the need to solve several forward multi-scale problems. To this end, we propose a numerical framework that exploits three key ingredients to mitigate these challenges: *(i)* computational homogenization, *(ii)* scientific machine learning based model order reduction (ML-MOR) – a two-tier deep network – of the micro-scale part, and *(iii)* parallelizable, derivative-free ensemble Kalman inversion. The performance of the proposed method is assessed on a non-linear hyper-elastic model. The obtained (physically-consistent) results confirm significant speed-ups upon using the surrogate micro-scale part, and yield inverse estimation in the multi-scale context with a sufficient accuracy.

Keywords: Kalman Inversion, Physics-informed Deep Learning, Model Order Reduction, Multi-scale Model

1 Introduction

We are interested in non-linear multi-scale inverse problems that arise in solid mechanics. Given only macro-scale boundary measurements, we wish to estimate a parameter field, in particular, the macroscopic distribution of the microscopic parameter, e.g., the radius of the micro-pores, as a function of macro-scale position.

The computational homogenization method (CHM), one of the most widely used homogenization techniques, divides the multi-scale model into macro-scale and (multiple) micro-scale simulations [1]. However, CHM is computationally very expensive. One way to reduce the computational cost of the forward multi-scale model is by using model order reduction (MOR). Reduced models of (nonlinear) problems have been developed using both projection-based MOR and scientific machine learning (ML) principles (see, e.g., [2]). However, the MOR techniques employed to reduce the complex model are often either intrusive or do not account for physical laws. We thus propose an offline- and online-efficient, non-intrusive, physics-informed two-tier deep network (TTDN) to reduce the computational cost of the micro-scale simulation.

Multi-scale inverse problems have been studied in the past using the combination of numerical homogenization, reduced basis approximations and Bayesian inversion or ensemble Kalman inversion (EnKI) techniques. Bayesian inversion requires first-order derivatives of the forward model w.r.t. the parameter of interest, which is difficult to obtain in the multi-scale context. To remedy this, derivative-free methods such as EnKI [3] are often preferred.

EnKI has also been shown to be successful in multi-scale inverse estimation, see, e.g., [4]. Here, we stride towards improving parameter estimation by replacing *(i)* a (linear) asymptotic homogenized model with a model based on computational homogenization, MOR and ML, and *(ii)* intrusive, conventional reduction with the non-intrusive, ML-based TTDN.

2 Mathematical framework

The forward multi-scale model, combined with the TTDN as a physics-informed ML-MOR, is depicted in Fig.1. The illustration shows that the surrogate micro-scale simulation is realized by the TTDN and the output $\mathbf{P}_{\mathrm{M}}$ is fed to the macro-scale simulation; see, e.g., [1].

Given boundary observations $\tilde{y}$, we aim to estimate parameter of interest $r(\boldsymbol{x}_{\mathrm{M}})$. Given a prior r_0, for the i-th particles inside the ensemble, EnKI provides the iteration for step n :

$$r_n^i = r_{n-1}^i + \mathbf{K}_n \cdot \left(\begin{bmatrix} r_0 & \tilde{y} \end{bmatrix}^T + \tilde{\epsilon}_n^i - \begin{bmatrix} r_{n-1}^i & \tilde{\mathcal{H}} \circ \mathcal{G}_r(r_{n-1}^i) \end{bmatrix}^T \right) + \alpha_n \hat{\epsilon}_n^i, \tag{1}$$

where $\mathcal{G}_r$ is the forward model, the Kalman gain $\mathbf{K}_n = \begin{bmatrix} \mathbf{I} & 0 \end{bmatrix} \cdot \mathbf{Q}_n \cdot (\mathbf{P}_n + \beta_n \mathbf{\Gamma})^{-1}$, $\mathbf{P}_n$ and $\mathbf{Q}_n$, respectively, are Monte Carlo estimates of the variance of $\mathcal{G}_r$ and covariance of $(\tilde{\mathcal{H}} \circ \mathcal{G}_r)$ and $\mathcal{G}_r$, $\tilde{\mathcal{H}}$ is the observation operator, $\mathbf{\Gamma}$ is the noise covariance, and $(\tilde{\epsilon}_n^i, \hat{\epsilon}_n^i)$ and (α_n, β_n), respectively, are independent Gaussian noise models and hyper-parameters; see, e.g., [3].

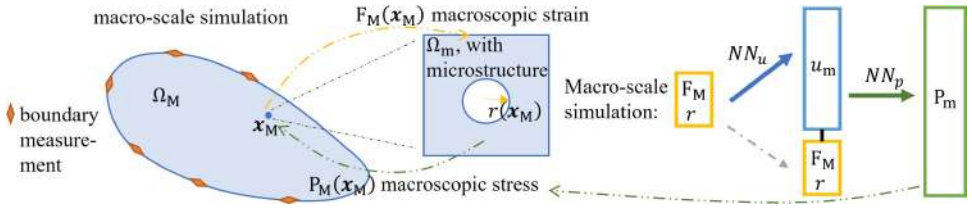


Figure 1: Paradigm of the computational model with boundary measurements.

3 Conclusions

Numerical results show that the ML-MOR leads to significant speed-ups versus the full order micro-scale simulation. The proposed framework, as a whole, yields high accuracy for the estimation of the microscopic parameter field.

References

[1] Geers, Marc GD, et al. Homogenization methods and multiscale modeling: nonlinear problems. Encyclopedia of computational mechanics second edition (2017): 1-34.

[2] Hesthaven J S, Ubbiali S. Non-intrusive reduced order modeling of nonlinear problems using neural networks. Journal of Computational Physics (2018): 55-78.

[3] Chada N, Tong X. Convergence acceleration of ensemble Kalman inversion in nonlinear settings. Mathematics of Computation (2022): 1247-1280.

[4] Abdulle A, Garegnani G, Zanoni A. Ensemble Kalman filter for multiscale inverse problems. Multiscale Modeling & Simulation (2020): 1565-1594.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Model order reduction for varying boundary optimal control problems

Maria Strazzullo* **and Fabio Vicini***

* Politecnico of Torino,
Department of Mathematical Sciences "Giuseppe Luigi Lagrange", Torino, Italy
e-mail:maria.strazzullo@polito.it, fabio.vicini@polito.it

Abstract: This talk introduces a novel model: varying boundary optimal control governed by partial differential equations (vbOCP($\boldsymbol{\mu}$)s). In this setting, specific parameters change *where* the boundary control acts on the system. The parametric nature of the problem naturally suits model order reduction. Indeed, vbOCP($\boldsymbol{\mu}$)s may represent several natural phenomena in geophysics and energy engineering, applied fields characterized by an increasing demand for fast and reliable simulations for several parametric instances in a data assimilation framework. However, vbOCP($\boldsymbol{\mu}$)s feature solutions with wave-like and transport phenomena. Classical model order reduction is not appropriate in this context. We propose tailored reduced approaches based on domain transformation or local basis functions. We compare them with standard proper orthogonal decomposition in terms of accuracy and efficiency. We test these techniques on two numerical settings with geometries (and, consequently, control action) of increasing complexity.

Keywords: Boundary optimal control, model order reduction, partial differential equations

1 Introduction

Varying boundary optimal control problems vbOCP($\boldsymbol{\mu}$) governed by parametric partial differential equations PDE($\boldsymbol{\mu}$)s are a natural extension of classical geometric boundary optimal control problems (OCP($\boldsymbol{\mu}$)s). The aim of a vbOCP($\boldsymbol{\mu}$) is to reach a desired state by means of an external variable acting on a portion of the boundary of the considered physical domain Ω (see Figure 1 for a schematic difference between vbOCP($\boldsymbol{\mu}$) and standard geometric OCP($\boldsymbol{\mu}$)s). The goal is achieved by means of a PDE($\boldsymbol{\mu}$)-constrained minimization problem. The main feature of an vbOCP($\boldsymbol{\mu}$) is the dependence from a specific parameter $\mu_u \in \mathbb{R}$ that changes *where* the control is acting, i.e. the portion of $\partial\Omega$ where the control is defined. The talk focuses on steady Neumann vbOCP($\boldsymbol{\mu}$)s. This model can be of interest in energy engineering and geophysics (baffled-heat exchangers or fractures moving and intersecting can be easily represented by vbOCP($\boldsymbol{\mu}$)). In these applied fields, there is a constant need for fast and reliable simulations for several parametric instances. Model order reduction (ROMs) is a valid option to deal with this task. The talk proposes (i) the novel vbOCP($\boldsymbol{\mu}$) model and (ii) an experimental analysis of ROMs approaches for vbOCP($\boldsymbol{\mu}$) based on tailored reduced strategies inspired from geometrical transformation and local basis generation. They were necessary, since vbOCP($\boldsymbol{\mu}$) present transport-like features and standard ROMs were not appropriate to deal with the proposed setting.

2 Problem formulation and reduced strategy

Let $\boldsymbol{\mu} = (\mu^1, \dots, \mu^{p-1}, \mu_u) \in \mathcal{P} \subset \mathbb{R}^p$, $p \in \mathbb{N}$ be a parameter in a parametric space, where $\mu_u \in \mathbb{R}$ defines the location of the boundary control $u \in U$ over $\partial\Omega$, where Ω is the spatial domain considered. We want to steer the state $y \in Y$ towards $y_\mathrm{d} \in L^2(\Omega_\mathrm{obs})$, with $\Omega_\mathrm{obs} \subseteq \Omega$ and U and Y suited Hilbert spaces. Namely, we solve the following minimization problem:

$$\min_{(y,u)\in Y\times U} \frac{1}{2}\|y - y_\mathrm{d}\|^2_{L^2(\Omega_\mathrm{obs})} + \frac{\alpha}{2}\|u\|^2_U, \tag{1}$$

constrained to an elliptic PDE($\boldsymbol{\mu}$) with homogeneous boundary conditions over $\Gamma_D \subset \partial\Omega$ and Neumann boundary conditions over $\Gamma_N = \partial\Omega \setminus \Gamma_D$. Γ_N is split into $\Gamma_C^{\mu_u}$ and $\Gamma_N^{\mu_u}$, i.e. the portions of $\partial\Omega$ where the control acts and where homogeneous Neumann conditions are applied, respectively (see Figure 1 for a representative domain representation).

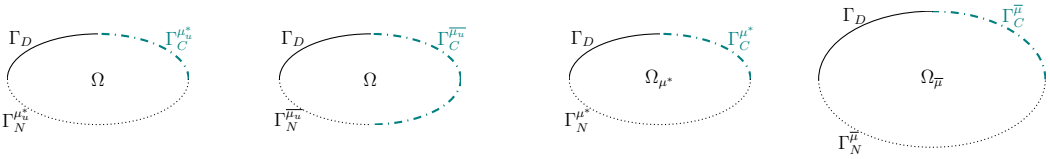


Figure 1: Schematic representation of a vbOCP($\boldsymbol{\mu}$) domain (extreme left and center left plots) and a standard geometric OCP($\boldsymbol{\mu}$) domain (center right and extreme right plots) for two different parametric instances.

For a vbOCP($\boldsymbol{\mu}$), the solution $y \in Y$ shows peaks that transport along the domain varying μ_u and thus we adapt reduced approaches based on nonlinear ROMs strategies to the proposed framework: we employ (i) Local Proper Orthogonal Decomposition (L-POD) and (ii) Geometric Recasting (Geo-R). For the description of the algorithms and the numerical results over geometries of increasing complexity, we refer the reader to [1].

3 Conclusions

Due to its nonlinear nature vbOCP($\boldsymbol{\mu}$)s are very complicated to reduce. The two proposed approaches outperform standard ROMs techniques, such as standard POD. For simple geometries Geo-R is the best choice in terms of accuracy and efficiency. However, for more complex domains Geo-R is not appropriate and L-POD represents a general and reliable strategy that shows benefits in terms of accuracy and computational costs with respect to standard POD.

References

[1] Strazzullo M and Vicini F. POD-based reduced order methods for optimal control problems governed by parametric partial differential equation with varying boundary control, submitted, 2023, https://arxiv.org/abs/2212.10654.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Parameter recovery for eigenvalue problems in linear elasticity

Cheng, Hanz Martin*

* School of Engineering Science, Lappeenranta–Lahti University of Technology, P.O. Box 20, 53851 Lappeenranta, Finland
email:hanz.cheng@lut.fi

Abstract: In this work, we explore some algorithms and techniques for recovering material parameters arising from eigenvalue problems in linear elasticity. This type of parameter recovery problem arises in the process of modal testing, where measurements on the eigenfrequencies of e.g. an engine rotor are provided. One of the main challenges we deal with is the fact that engine rotors are anisotropic, and that inverse problems involving anisotropic linear elasticity eigenvalue problems is a relatively new field of research.

Keywords: linear elasticity, eigenvalue problem, inverse problem, anisotropy

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Ensemble Kalman–Bucy filters for finite and infinite dimensional signals

Sebastian Ertel*

*Institut für Mathematik, Technische Universität Berlin, Germany
e-mail: ertel@math.tu-berlin.de

Abstract: Ensemble Kalman–Bucy filters (EnKBFs) are an important tool in Data Assimilation that aim to approximate the posterior distribution for continuous time filtering problems using an ensemble of interacting particles.
In this talk we first derive a (deterministic) mean-field EnKBF for finite dimensional, nonlinear, continuous time filtering problems as a constant gain approximation to the optimal filter. Other well known versions of the EnKBF are then obtained by replacing Brownian motions with deterministic inflation terms and vice versa.
We then prove the well posedness of this class of mean-field equations via a combination of a fixed point and a partial stopping argument.
Next we investigate the mean-field EnKBF when the signal is given by a nonlinear SPDE, i.e. for infinite dimensional signals. In this case proving the well posedness requires an adaptation of the fixed point argument, which makes use of the robustness of the law of total variance with respect to the observation function.
Finally, if time permits, we discuss the analysis of the approximating particle system and a propagation of chaos result.

Keywords: Data Assimilation, Ensemble Kalman–Bucy filter, Feedback Particle Filter, SPDEs, correlated noise, , propagation of chaos

References

[1] Ertel S, Stannat W. Analysis of the Ensemble Kalman–Bucy Filter for correlated observation noise. arxiv: 2205.14253.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

An IMEX-DG solver for the compressible Navier-Stokes equations for non-ideal gases

Giuseppe Orlando*, Paolo Francesco Barbante* and Luca Bonaventura*

* MOX, Dipartimento di Matematica
Politecnico di Milano
Milan, Italy

Abstract: We propose an efficient, accurate and robust IMEX solver for the compressible Navier-Stokes equations describing non-ideal gases with general cubic equation of state and Stiffened-Gas EOS. The method is based on an h-adaptive Discontinuous Galerkin spatial discretization and on an Additive Runge Kutta IMEX method for time discretization. It is specifically tailored for low Mach number applications and allows to simulate this kind of regimes at a significantly reduced computational cost. The method has been implemented in the framework of the *deal.II* numerical library, whose adaptive mesh refinement capabilities are employed to enhance efficiency and regions of interest. Refinement indicators appropriate for real gas phenomena will be introduced. A number of numerical experiments on classical benchmarks for compressible flows, including test cases for atmosphere dynamics without and with orography, and their extension to real gases demonstrate the properties of the proposed method. Suitable extensions for two-phase flows will be also discussed.

Keywords: Navier-Stokes equations, Discontinuous Galerkin methods, Adaptive Mesh Refinement, Atmosphere dynamics, Non-ideal gases

1 Introduction

The use of implicit and semi-implicit methods has a long tradition in low Mach number flows, see e.g [4] and the references therein. In this work, we propose a discretization approach for the equations of non-ideal compressible gas dynamics [1]. The goal is to derive a method that can then be easily extended to handle two-phase compressible flows, where a number of coupling and forcing terms arise that cannot be dealt with efficiently by straightforward application of conventional solvers. The proposed method is implemented in the numerical library *deal.II* [3]. This software also provides h-refinement capabilities that are exploited by the proposed method. For the specific case of real gases, novel physically based refinement criteria have been proposed and tested.

2 Models and results

Let $\Omega \subset \mathbb{R}^d, 2 \leq d \leq 3$ be a connected open bounded set with a sufficiently smooth boundary $\partial\Omega$. We consider the classical unsteady compressible Navier-Stokes equations in flux form. The above equations must be complemented by an equation of state (EOS) for the compressible fluid. A classical choice is that of an ideal gas. An example of non-ideal gas equation of state is given by the general cubic equation of state that reads as follows. We have shown that, under specific assumptions, the quantity $\beta = \log(T) - 2\frac{R_g}{c_v}\,\mathrm{atanh}\,(2\rho b - 1)$ is constant for

isentropic processes and can be therefore used for mesh adaptation procedures. Here T is the absolute temperature, R_g is the specific gas constant, c_v is the specific heat at constant volume, ρ is the density and b is a suitable parameters that characterizes the gas behaviour. The last example of non-ideal gas considered is represented by the Stiffened Gas equation of state (SG-EOS). We use a flexible space discretization and a second order implicit-explicit (IMEX) time discretization, combined to obtain an efficient method for compressible flow of real gases at low to moderate Mach number. More specifically, following [4], we couple implicitly the energy balance to the momentum one, while treating the continuity equation in an explicit fashion. Moreover, as commonly done in numerical models for atmospheric physics, we split the hyperbolic part of the problem from the diffusive terms, which are treated using the implicit part of the IMEX scheme employed for the hyperbolic terms.

3 Conclusions

We have proposed an efficient, h-adaptive IMEX-DG solver for the compressible Navier-Stokes equations with non-ideal EOS. The resulting method is implemented in the framework of the numerical library *deal.II* and exploits its h-adaptive capabilities on the basis of physically based adaptation criteria that have been proposed specifically for the non-ideal gas case. A number of numerical experiments,including test cases for atmosphere dynamics without and with orography, validate the proposed method and show its potential for low Mach number problems. Moreover, possible extensions to two-phase flows have been discussed.

4 Acknowledgements

This work was supported by the ESCAPE-2 project, European Union's Horizon 2020 Research and Innovation Programme (Grant Agreement No. 800897).

References

[1] G. Orlando and P. F. Barbante and L. Bonaventura. An efficient IMEX-DG solver for the compressible Navier-Stokes equations for non-ideal gases. Journal of Computational Physics, 471:111653, 2022

[2] G. Orlando and T. Benacchio and L. Bonaventura. An IMEX-DG solver for atmospheric dynamics simulations with adaptive mesh refinement. arXiv preprint arXiv:2210.07898, 2022.

[3] D. Arndt and W. Bangerth and M. Feder and M. Fehling and R. Gassmöller and T. Heister and L. Heltai and M. Kronbichler and M. Maier and P. Munch and J.P. Pelteret and S. Sticko and B. Turcksin and D. Wells. The deal II library, version 9.4.. Journal of Numerical Mathematics, 30:231-246, 2022.

[4] M. Dumbser and V. Casulli. A conservative, weakly nonlinear semi-implicit finite volume scheme for the compressible Navier-Stokes equations with general equation of state. Applied Mathematics and Computation, 272:479-497, 2016.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A high-order continuous Lagrange–Galerkin method for compressible flows

Manuel Colera*, Jaime Carpio* and Rodolfo Bermejo †

* Departamento de Ingeniería Energética
Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid
Madrid, Spain

† Departamento de Matemática Aplicada a la Ingeniería Industrial
Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid
Madrid, Spain

Abstract: We present a novel Lagrangian–Eulerian scheme for the resolution of two-dimensional compressible and inviscid flows. The scheme considers arbitrary-order continuous space discretizations on unstructured triangular meshes, as well as arbitrary-order implicit–explicit Runge–Kutta time marching schemes. The method preserves mass, momentum and total energy as long as the integrals in the formulation are computed exactly. The recent model proposed by Brenner [1] for viscous flows is employed to define the operators needed to stabilize the continuous Galerkin formulation. The method has been tested on several benchmark problems using a fourth-order time-marching formula and up to fifth-order elements, showing good accuracy both for smooth and discontinuous solutions.

Keywords: finite element method, compressible flows, high-order methods, conservative methods

1 Formulation

In this work, we focus on the Euler equations for compressible and inviscid flows,

$$\partial_t u_I + \partial_j \left(v_j u_I\right) = \partial_j \left(f_{Ij}\right), \tag{1}$$

with $\partial_t \equiv \partial/\partial t$, $\partial_j \equiv \partial/\partial x_j$, t the time, $\mathbf{x}$ the position vector, $\mathbf{u} = [\rho, m_1, m_2, \mathcal{E}]^T$ the vector of conservative variables, $\mathbf{f} = \mathbf{f}(\mathbf{u})$ the pressure flux matrix, $f_{1,j} = 0$, $f_{1+i,j} = -p\delta_{ij}$, $f_{4,j} = -pv_j$, ρ the density, $\mathbf{v}$ the velocity, $\mathbf{m} = \rho\mathbf{v}$ the momentum per unit of volume, $\mathcal{E} = p/(\gamma-1)+\rho v_i v_i/2$ the total energy per unit of volume and γ the adiabatic constant of the gas. We adopt Einstein's summation convention, with uppercase and lowercase indices varying from 1 to 4 and from 1 to 2, respectively.

The so-called *weak Lagrange–Galerkin formulation* [2] associated with Eq. (1) is

$$\partial_t \int_{\Omega_f} u_I \psi \,\mathrm{d}\Omega = -\int_{\Omega_f} f_{Ij}\partial_j\psi \,\mathrm{d}\Omega + \int_{\partial\Omega_f} f_{Ij}\psi n_j \,\mathrm{d}\sigma, \quad \forall\psi \in V, \tag{2}$$

where $\Omega_f(t) := \left\{\mathbf{x}(t) \in \mathbb{R}^2 : \mathrm{d}\mathbf{x}/\mathrm{d}t = \mathbf{v}(\mathbf{x}(t), t)\right\}$ is a domain that moves with the fluid, $\mathbf{n}$ is the outward normal vector to the boundary $\partial\Omega_f$, and $\psi(\mathbf{x}, t)$ is a continuous test function such that remains constant along the trajectories of the fluid particles, i.e., $\mathrm{D}_t\psi := \partial_t\psi + v_j\partial_j\psi = 0$.

Following [3], Eq. (2) is first discretized in space with a multiscale finite element method. The mesh moves with $\Omega_f(t)$ and therefore the method is Lagrangian. Then, we march in

time with an implicit–explicit Runge–Kutta (RK) method. Specifically, for each stage of the RK method we perform the following steps: (i) the mesh is displaced with the explicit part, (ii) Eq. (2) is solved as is (without any stabilization terms) with the explicit part, and hence we obtain a non-stabilized solution $\mathbf{u}_*$, (iii) the latter is post-processed to detect the discontinuities and to compute an artificial-viscosity based stabilization operator, and (iv) Eq. (2) is equipped with the stabilization operator and solved with the implicit part of the RK method to yield a smooth solution $\mathbf{u}_h$. Periodically, $\mathbf{u}_h$ is remapped from the moving mesh to a fixed (reference) mesh to avoid mesh distortion problems.

2 A numerical example

To check the accuracy of the method, we have solved several benchmark problems. In Fig. 1 we show the results for the so-called shock–vortex interaction problem [4].

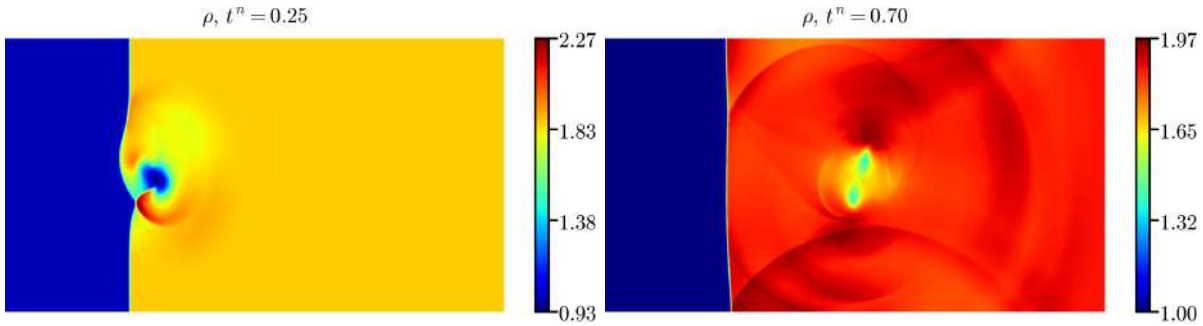


Figure 1: Numerical solution of the shock–vortex interaction problem for fifth-order elements and mesh size $h \simeq 0.01$.

Acknowledgements

This research has been partially funded by project PGC-2018-097565-BI00 from the "Ministerio de Ciencia, Innovación y Universidades" of Spain and the European Regional Development Fund, and by the FPU16/05509 grant to M. Colera from the "Ministerio de Ciencia, Innovación y Universidades" of Spain.

References

[1] Howard Brenner. Fluid mechanics revisited. *Physica A: Statistical Mechanics and its Applications*, 370(2):190–224, October 2006.

[2] Manuel Colera, Jaime Carpio, and Rodolfo Bermejo. A nearly-conservative high-order Lagrange–Galerkin method for the resolution of scalar convection-dominated equations in non-divergence-free velocity fields. *Computer Methods in Applied Mechanics and Engineering*, 372:113366, December 2020.

[3] Manuel Colera, Jaime Carpio, and Rodolfo Bermejo. A nearly-conservative, high-order, forward Lagrange–Galerkin method for the resolution of compressible flows on unstructured triangular meshes. *Journal of Computational Physics*, 467:111471, October 2022.

[4] Audrey Rault, Guillaume Chiavassa, and Rosa Donat. Shock-Vortex Interactions at High Mach Numbers. *Journal of Scientific Computing*, 19(1):347–371, December 2003.

[5] Homer F. Walker and Peng Ni. Anderson Acceleration for Fixed-Point Iterations. *SIAM Journal on Numerical Analysis*, 49(4):1715–1735, January 2011.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Simulation of Centrifugal Buoyancy-Induced Flow in Sealed and Open Rotating Compressor Cavities Using the Lattice-Boltzmann Method

Paul Werner[*†‡], **Jean-François Boussuge**[*], **Christophe Scholtes**[†], **Pierre Sagaut**[‡]

[*] Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS)
Toulouse, France
e-mail: werner@cerfacs.fr, boussuge@cerfacs.fr

[†] Safran Aircraft Engines (SAE)
Moissy-Cramayel, France
e-mail: christophe.scholtes@safrangroup.com

[‡] M2P2 UMR 7340
Aix-Marseille Université (AMU)
Marseille, France
e-mail: pierre.sagaut@univ-amu.fr

Abstract: The flow structure within the cavities between each rotor disks of the high-pressure compressor is inherently unsteady due to both forced and natural convection phenomena induced respectively by the cooling axial through-flow and by the opposing effects of the centrifugal force field and the large temperature gradients. This talk presents an approach based on a hybrid Lattice-Boltzmann Method (LBM) capable of modeling such buoyancy-driven flows. A local rotating reference frame model is combined with a segregated thermal LBM to simulate the rotation of perfect gases by considering centrifugal and Coriolis force terms. Then, a mass-conserving boundary treatment that handles surface curvature allows for the accurate prediction of the Nusselt number on the disks. Finally, a modified mesh refinement strategy based on [5] enables the extension of the simulations to higher Rayleigh numbers. Coupled with a Large Eddy Simulation (LES) turbulence model, the proposed approach is able to recover flow and heat transfer mechanisms of sealed [6] and open [1] rotating compressor cavity rigs covering a large range of Rayleigh numbers ($10^6 - 10^{14}$). It compares well with published numerical studies from other solvers, producing precise results for a simulation time that is shorter by an order of magnitude. The proposed approach is thus a promising method for the simulation of turbomachinery cooling circuits.

Keywords: Buoyancy-driven flows, Heat transfer, Compressor cavities, Large Eddy Simulation, Lattice-Boltzmann Method.

References

[1] D. E. Bohn, G. N. Deutsch, B. Simon, and C. Burkhardt, Flow Visualisation in a Rotating Cavity With Axial Throughflow, in Volume 3: Heat Transfer; Electric Power; Industrial and Cogeneration (American Society of Mechanical Engineers, Munich, Germany, 2000), p. V003T01A084.

[2] Q. Tan, J. Ren, and H. Jiang, Prediction of Flow Features in Rotating Cavities With Axial Throughflow by RANS and LES, in (American Society of Mechanical Engineers Digital Collection, 2010), pp. 1173–1181.

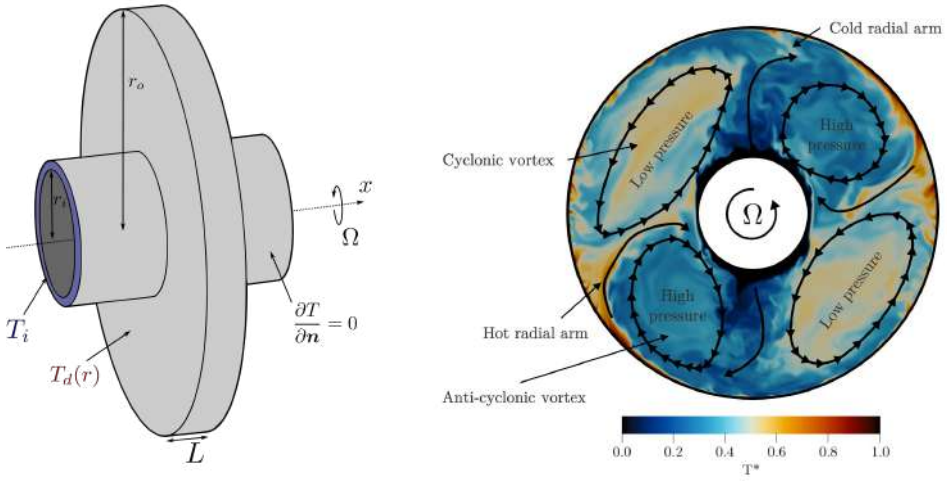


Figure 1: *Left*: Scheme of the rotating open cavity rig of [1] where an axial throughflow of air of temperature T_i is used to cool non-uniformly heated disks at a temperature $T_d(r)$. *Right*: Non-dimensional temperature field T at the mid-section of the cavity.

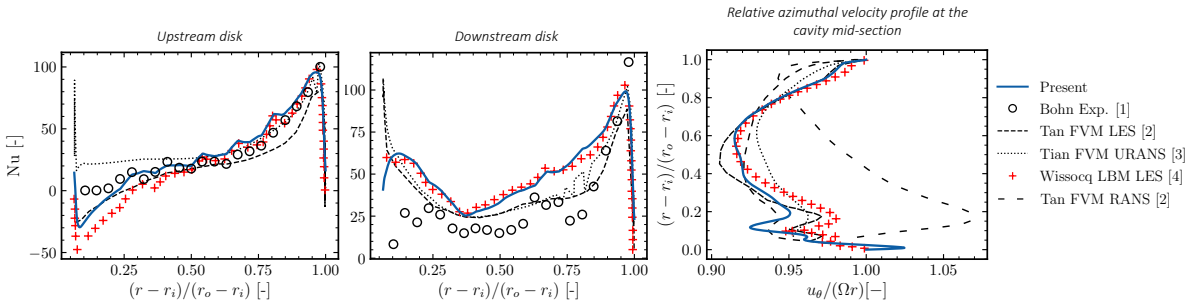


Figure 2: Radial Nusselt number profiles of both upstream (*left*) and downstream (*middle*) disks and relative azimuthal velocity profile at the cavity mid-section (*right*) against experimental data of [1] and numerical studies from other solvers [2, 3, 4].

[3] S. Tian and Y. Zhu, Disk Heat Transfer Analysis in a Heated Rotating Cavity With an Axial Throughflow, in Volume 4: Heat Transfer, Parts A and B (American Society of Mechanical Engineers, Copenhagen, Denmark, 2012), pp. 2191–2199.

[4] G. Wissocq, Investigation of Lattice Boltzmann Methods for Turbomachinery Secondary Air System Simulations, Aix-Marseille Université, 2019.

[5] T. Astoul, G. Wissocq, J.-F. Boussuge, A. Sengissen, and P. Sagaut, Lattice Boltzmann Method for Computational Aeroacoustics on Non-Uniform Meshes: A Direct Grid Coupling Approach, Journal of Computational Physics 447, 110667 (2021).

[6] D. Bohn, E. Deuker, R. Emunds, and V. Gorzelitz, Experimental and Theoretical Investigations of Heat Transfer in Closed Gas-Filled Rotating Annuli, Journal of Turbomachinery 117, 175 (1995).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A mixed Lagrangian-Eulerian formulation for Particle Finite Element Method

Cheng Fu[1], **Massimiliano Cremonesi**[1] **Umberto Perego**[1]

[1] Department of Civil and Environmental Engineering (DICA)
Politecnico di Milano
Milan, Italy
e-mail: cheng.fu@polimi.it

Abstract: Fluid flows interacting with highly deformable structures and free surfaces are present in many engineering problems and methods for their solution attract considerable attention in many engineering fields. There are many numerical methods available in the literature for fluid simulations. Among them, the Particle Finite Element Method (PFEM) is a mesh-based Lagrangian approach, particularly suited for fluid modelling with rapid changes in the domain topology. The PFEM represents a powerful numerical tool for solving Fluid-Structure Interaction (FSI) problems involving large structure deformations and fluid free-surface flows, since fluid boundaries and FSI interfaces are tracked naturally by the position of the mesh nodes. However, an Eulerian formulation is more convenient for solving fluid problems characterized by confined portions of the domain with a fixed geometry or by non-homogeneous boundary conditions on velocities. In this work, a mixed Lagrangian-Eulerian approach is presented with the aim of exploiting the advantages of both formulations. According to the proposed method, nodes on the fluid free-surface and on the FSI interface are analysed in the Lagrangian framework, while the remaining nodes can be either Eulerian or Lagrangian. Furthermore, an algorithm to detect runtime the transition zone between the two kinematic descriptions for FSI problems has been introduced to increase the efficiency of the method.

Keywords: Mixed Lagrangian-Eulerian, Particle Finite Element method (PFEM), Fluid Structure Interaction (FSI), Explicit Dynamics

1 Introduction

Fluid flows and Fluid-Structure Interaction (FSI) problems characterized by fast domain evolution and large structural deformations are present in problems of great interest in many research areas, such as civil, aerospace and biomedical engineering.

The motion of viscous fluids is governed by the Navier-Stokes equations that can be formulated either in the Eulerian or in the Lagrangian framework. In the former approach, a fixed control volume in which the material flows is considered for the fluid analysis. When a mesh-based approach is used, the computational mesh remains unchanged in time and this facilitates the treatment of fixed boundaries with prescribed fields. However, the free surface and FSI interface tracking does not occur in a natural way in the Eulerian description and ad-hoc techniques are required. By contrast, in the Lagrangian approach, the computational mesh is attached to the material and the position of mesh nodes is updated according to the fluid particles movement. As a consequence, the mesh undergoes excessive distortion in large-deformation problems and frequent remeshing is required. When the mesh problem is properly treated, the latter approach represents an efficient tool for simulating fluid and FSI

problems involving free surface flows and highly deformable structures.

Recently, Lagrangian mesh-based methods have been successfully employed for solving fluid flow problems thanks to the improvements in mesh generation algorithms. The Particle Finite Element Method (PFEM) is a Lagrangian finite element approach characterized by runtime mesh regeneration performed when the current one becomes too distorted due to fluid movement. The PFEM was initially introduced for solving free surface flows [1] but soon after it showed the ability to simulate FSI problems[2], granular[3] and thermal coupled analyses[4].

In this work, a mixed Lagrangian-Eulerian kinematic model for PFEM is presented. The proposed technique divides the domains into Eulerian and Lagrangian regions in order to fully exploit their advantages. The Lagrangian approach is used close to the fluid free surfaces and fluid-structure interfaces, whereas the Eulerian approach is adopted elsewhere. The proposed method is also extended to FSI problems by introducing a rectangular (in 2D) remeshing region enclosing the structure. Inside this region, nodes are treated as Lagrangian to facilitate interface tracking, while the remaining nodes are set to be Eulerian. In order to fit the solid body during the motion, the position and space extension of the remeshing region are updated in the analysis, e.g. when the structure reaches the interfaces separating Lagrangian from Eulerian regions.

2 Conclusions

A mixed Lagrangian and Eulerian multi-domain formulation for PFEM is presented in this work. This approach aims to exploit the advantages of the two kinematic descriptions for the treatment of fluids and FSI problems in explicit PFEM. Lagrangian description is conveniently adopted in regions where large changes in domain topology are expected, such as zones close to free surfaces and FSI interfaces. By contrast, the Eulerian framework is considered in regions where no significant evolutions of the domain are expected or where complex boundary conditions are imposed.

References

[1] Oñate E, Idelsohn SR, Del Pin F, Aubry R. The particle finite element method—an overview. International Journal of Computational Methods, 1(02):267-307,2004.

[2] Idelsohn SR, Oñate E, Del Pin F,Calvo N. Fluid-structure interaction using the particle finite element method. Computer methods in applied mechanics and engineering, 195(17-18):2100-2123,2006.

[3] Cremonesi M, Ferri F, Perego U. A basal slip model for Lagrangian finite element simulations of 3D landslides. International Journal for Numerical and Analytical Methods in Geomechanics, 41(1):30-53,2017.

[4] Oñate E, Franci A, Carbonell JM. A particle finite element method (PFEM) for coupled thermal analysis of quasi and fully incompressible flows and fluid-structure interaction problems. Numerical Simulations of Coupled Problems in Engineering, 129-156, 2014.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Multipoint Shape Optimization of a Pump-Turbine Using the Adjoint Method

Huscava Alexander*, Semlitsch Bernhard†

Institute of Energy Systems and Thermodynamics (IET)
Faculty of Mechanical and Industrial Engineering, Vienna University of Technology
Vienna, Austria
e-mail: * alexander.huscava@tuwien.ac.at † bernhard.semlitsch@tuwien.ac.at

Abstract: Improving hydroelectric facilities becomes essential with more fluctuating energy sources, i.e. solar and wind energy, in the energy grid. Pumped-storage hydropower balances the electricity generation with the demand. The wide operating range required for such applications challenges the pump-turbine design. We aim to optimize the shape of the pump-turbine runner blades such that the overall efficiency of the pump-turbine at multiple operating points increases. Therefore, computational fluid dynamics and an adjoint-based optimization approach are employed. Adjoint-based gradient optimization allows efficient blade shape optimization with many degrees of freedom. The optimization results show that the power input required in pump mode can be decreased significantly within a few design iterations. The blade shape alters mainly at the trailing edge, which moves towards the center of rotation. Combining multiple optimized shapes into a single pump-turbine design for a flexible operating range will be discussed.

Keywords: Hydro Power, Computational Fluid Dynamics, Adjoint Shape Optimization

1 Introduction

Due to the rapid expansion of fluctuating renewable power sources, flexible pumped hydro storage has become increasingly important. Therefore, improving the pump-turbine performance over a wide operating range is an important field of research we want to contribute. Our aim is to increase the overall efficiency for multiple operating points of pump-turbines with shape optimization using computational fluid dynamics and adjoint-based gradient optimization. Adjoint optimization has the advantage that the calculation time scales independently from the number of design variables [1]. This is advantageous for complex geometries, which are often found in turbomachinery.

2 Methods

The runner blades of a pump-turbine are optimized using the software package DAFoam (Discrete Adjoint Foam) [1]. The flow through a blade passage is numerically simulated while applying periodic boundary conditions. The runner interfaces with the static components are modeled as mixing planes, and the data is transferred from the simulation of the whole assembly. The inflow and outflow boundary conditions and the rotating speed are set to match the experimental setup. The procedure depicted in figure 1 is applied to obtain the optimized shape. The steady-state, incompressible solver simpleFoam (OpenFOAM) with the Spallart-Allmaras turbulence model is used to compute the flow solutions for the

operating points. Then the adjoint optimization algorithm calculates the adjoint-gradient and changes the design variables to minimize the combined objective function. In this implementation, the design variables are free-form deformation points. These points are mapped on the runner blade surfaces and can be moved by the algorithm. The required moment to turn the rotor is used as the objective function. In order to decrease the power input, the moment should decrease while mass flow, rotation speed, and pressure ratio stay constant. Finally, the optimized runner geometry is reinserted into the whole pump-turbine assembly to verify the outcomes.

3 Results

Results for two exemplary operating points in pump mode show a decrease of 10.5 % for the moment coefficient after five design iterations. Since $P = M \cdot \omega$ and ω are constant at operating points, the required power to operate the pump-turbine drops proportionally. The blade shape is primarily changing at the trailing edge, moving closer to the rotation axis. Figure 2 shows the shape transformation for different cross-sections across the blade's span.

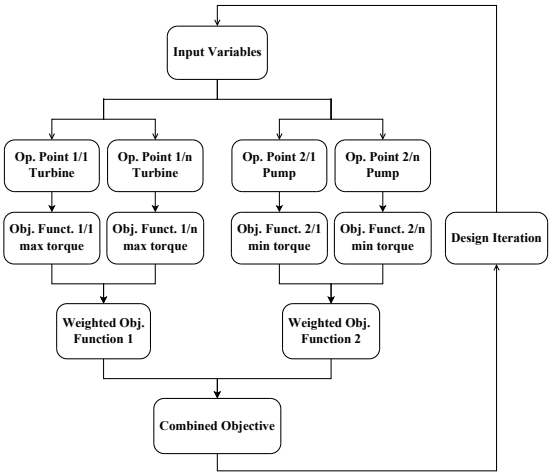


Figure 1: Optimization flow chart

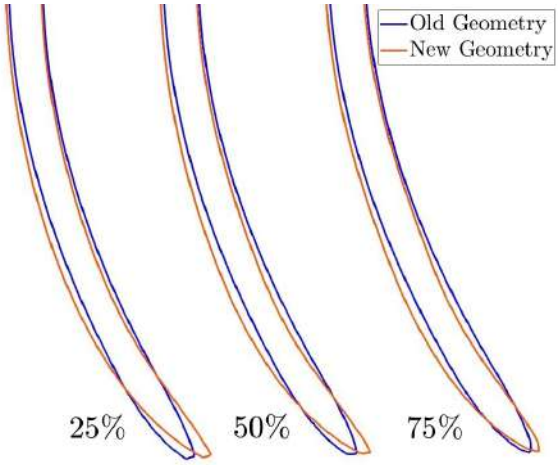


Figure 2: Blade change at the trailing edge

4 Discussion

The initial optimization results are auspicious. However, more design optimization iterations are needed to reach full convergence, which could not be achieved due to resource constraints. Therefore, better results are expected using high-performance computing clusters. More operating points in pump and turbine modes will be considered. The final goal is a pump-turbine design for flexible use with rapidly changing operating points and an overall high efficiency.

References

[1] Ping He, Charles A. Mader, Joaquim R.R.A. Martins, Kevin J. Maki. DAFoam: An open-source adjoint framework for multidisciplinary design optimization with OpenFOAM. AIAA Journal, 58:1304-1319, 2020. https://doi.org/10.2514/1.J058853

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Experimentally validated 3-D coupled model of freezing in small-scale freeze-dryer

Edyta Piechnik*†, Jacek Smolka*, Michal Palacz*, Ignat Tolstorebrov†, Trygve M. Eikevik†, Michal Stebel*, Michal Haida*, Andrzej J. Nowak*, Jakub Bodys*

* Department of Thermal Technology (ITT)
Silesian University of Technolog
Gliwice, Poland
e-mail: edyta.piechnik@polsl.pl

†Department of Energy and Process Engineering (EPT)
Norwegian University of Science and Technology
Trondheim, Norway

Abstract: This paper discusses an experimentally validated 3-D CFD model of the food freezing process in a household freeze-dryer with forced air circulation. The coupled model consists of three sub-models to simulate simultaneously the chamber cooling, product freezing add evaporator operation. Moreover, an analysis of airflow distribution for various internal geometry of the chamber components was performed. That analysis included the variation of the air fan size and position and the distance between the shelves and freeze-dryer doors. The computational results helped to redesign the interior of the investigated chamber and guarantee a more uniform air distribution. This directly affected the reduction of discrepancies in the freezing time of samples placed on different shelves. The freezing time for the bottom and top shelves for the optimal design was equal to 34 and 46 min, while it was equal to 106 and 128 min respectively for the original design. It should be highlighted that the proposed numerical tool and multivariant approach can be easily adapted to improve the design of various freeze-drying systems with the integrated ice trap. Hence, the utilisation of that CFD model will help to reduce the freeze-drying time and energy consumption for numerous applications.

Keywords: Food freezing, Cold-chain, Numerical modeling, Coupled solution, Freeze-drying

1 Introduction

In this study, the coupled 3-D CFD model of the freeze-dryer chamber was developed to analyse the freezing process and airflow inside that device. The integration of the freezing and freeze-drying processes in one unit is a novel concept that helps to make the system compact, cheap and flexible. Due to the complexity of the freeze-drying chamber, the developed model included a number of multiscale processes such as air fan operation, unsteady operation of the evaporator, and freezing process inside the food sample. In consequence, the model was divided into a number of sub-models and then coupled with the in-house developed script. The model was validated using the measured temperatures at the centre of the food samples located on two different shelves inside the storage chamber. The entire freezing process can be divided into three characteristic stages, namely: the cooling phase (to the initial freezing point of about -1.8 °C), the phase change phenomenon, and the cooling of the frozen sample to a temperature of about -40 °C.

2 Methodology

The research strategy consisted of several steps. First, the experimental investigation of the reference device to collect data for validation was performed. Next, the 3-D CFD model of the freeze-dryer chamber for airflow analysis was prepared. Using the mentioned model, various variants of the internal design of the chamber in order to improve the uniformity of air distribution were simulated. The modifications focused on three variables, namely fan area and number, and distance between the edge of the shelves and the appliance door. The next step covered the development and validation of a coupled 3-D CFD model for food freezing simulations. In the end, model accuracy was determined using relative root mean square error (RRMSE) and coefficient of determination (R^2).

3 Results

The results of the validation suggested that the freezing process was properly modeled. RRMSE of the CFD model was established at the level of 3.5 % for the product located on the top shelf and 19 % for the product located on the middle shelf. Moreover, R^2 was equal to 0.989 and 0.988, for the top and middle shelves, respectively.

Based on the results of the multi-variant analysis, the solution with two fans placed one above the other and with a distance of 0.05 m between the shelves and the door of the device turned out to be the most advantageous. A comparison of this conceptual solution with the basic case is presented in Fig. 1.

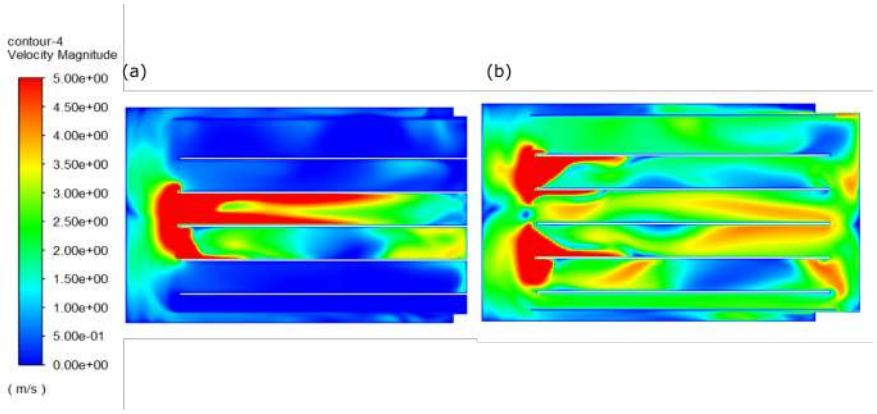


Figure 1: Comparison of velocity magnitude fields for (a) reference case and (b) prototype case

Fig. 1 (a) represents the reference device geometry. For most of the shelves, the velocity magnitude was around 1 m·s^{-1}, except for the middle one in front of which the fan is located. The cross-section presented in Fig. 1 (b) presents results for a prototype solution. In this case, on almost each of the shelves velocity magnitudes reached about 3 m·s^{-1}. The freezing time on individual shelves, determined using Pham's method [1] was 46 minutes, 39 minutes, and 34 minutes for the top, middle, and bottom shelves for the prototype case, respectively. While in the reference case, the freezing times on the same shelves were equal to 128 min, 27 min, and 106 min, respectively.

4 Conclusions

Based on the presented numerical results, a new design of the internal chamber of the freeze-dryer was proposed, taking into account two fans and a gap between shelves and the appliance door of 0.05 m. Providing a bigger gap between the shelves and the appliance door allowed air to flow to the front of the chamber and return to the other shelves more effectively. The arrangement of the shelves was kept the same as in the reference device. Such organisation of the chamber interior geometry allowed for the reduction of the difference in freezing time between the compared products. In the next steps, the prepared and validated coupled CFD model will be used to redesign the freeze-dryer chamber and adapt it for the microwave heating system.

5 Acknowledgements

Financial assistance was supported by the Norway Grants, in the frame of the Applied Research Programme-Poland.

References

[1] Q. Pham, A fast, unconditionally stable finite-difference scheme for heat conduction with phase change, International Journal of Heat and Mass Transfer 28 (11) (1985) 2079 – 2084.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Effect of Vapour Bubble Initial Displacement on Droplet Impact onto Liquid Films

Daniel Vasconcelos*, André Silva*, Jorge Barata*

*AEROG/LAETA
Universidade da Beira Interior
Covilhã, Portugal
e-mail: daniel.vasconcelos.rodrigues@ubi.pt

Abstract: Heat and mass transfer mechanisms regarding droplet impact have been extensively studied for dry surfaces, and in terms of droplet evaporation/combustion during free-fall. On the contrary, the droplet impact phenomena onto heated liquid films is a topic overlooked in the literature and requires further understanding in terms of hydrodynamics and phase change. Therefore, this work focuses on numerically simulating droplet impact onto liquid films in the presence of vapour bubbles. The crown height, diameter and overall development are analysed as a function of the position of the bubble related to the axis of symmetry. Results show that the crown overall growth is affected if the vapour bubbles detach and contact the crown wall. The size of the vapour bubbles also influences the detachment from the surface.

Keywords: Droplet Impact, Numerical Model, Bubble Formation, Crown Disintegration

1 Introduction

The mathematical and numerical comprehension of multiphase flows are topics both extensively studied and far from understood. Specifically, the droplet impact phenomena and associated interfacial phenomena, such as surface tension, evaporation and condensation, are difficult to implement in euler-euler formulations, along with the underlying fluid dynamics of the droplet-liquid film interactions. These are found in practical applications such as internal combustion engines, heat exchangers, and electronic cooling devices, in which temperature plays a major role. If a heated surface is covered by a liquid film, local boiling effects will occur, leading to the appearance of vapour bubbles on the impact surface, which affect the impact phenomena.

The influence of the bubble size and spacing on the crown formation and disintegration has been studied in previous works [1]. However, the initial bubble displacement (which refers to the vapour bubble closest to the symmetry axis) was not varied during the experiments, which may be an important factor in determining the crown overall development. Therefore, this work focuses on numerically simulating droplet impact onto liquid films in the presence of vapour bubbles, in which the first bubble positioning in relation to the axis of symmetry is varied.

2 Numerical Model

The numerical model consists on solving the Navier-Stokes equations coupled with the VOF method for liquid-gas interface tracking, which has been fully detailed [1]. Basilisk [2] was the

open-source software adopted for the numerical simulations. Figure 1 displays a schematic of the physical setup. A single droplet impacts vertically onto a liquid film of a certain thickness. Vapour bubbles are positioned in the impact surface to represent boiling effects. These are defined by their diameter, D_v, spacing, x_v, and the positioning of the first bubble, x_s, meaning the displacement of the vapour bubble in relation to the axis of symmetry. This last parameter will be modified to verify its influence on the impact outcome.

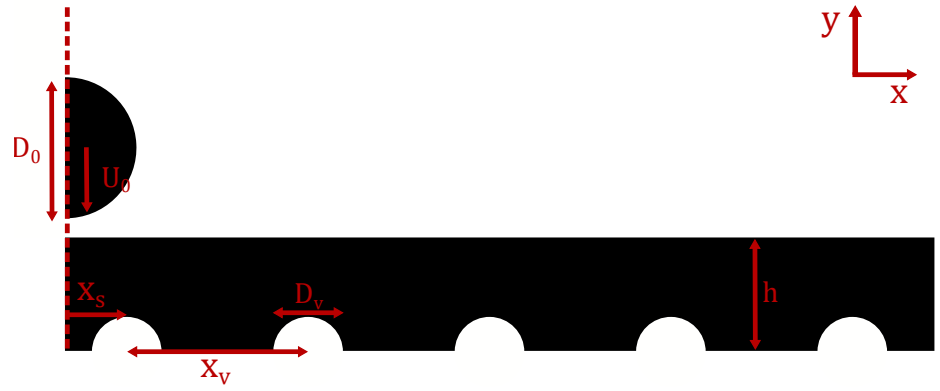


Figure 1: Numerical setup: x_s - Initial vapour bubble displacement from axis of symmetry; D_0 - Droplet diameter; U_0 - Droplet impact velocity; D_v - Vapour bubble diameter; x_v - Vapour bubble spacing; h - Liquid film thickness.

3 Conclusions

Numerical simulations of droplet impacting onto a heated liquid film in the presence of vapour bubbles were performed. Results show that the crown overall growth is affected if the vapour bubble detaches from the impact surface and contacts the liquid crown wall, leading to disintegration. The size of vapour bubbles is also a factor, as smaller bubbles tend to stick to the impact surface, not disturbing the crown walls.

4 Acknowledgements

The present work was performed under the scope of Aeronautics and Astronautics Research Center (AEROG) of the Laboratório Associado em Energia, Transportes e Aeronáutica (LAETA) activities, supported by Fundação para a Ciência e Tecnologia (FCT) through the project number UIDB/50022/2020 and by the Ph.D. scholarship with the reference SFRH BD/143307/2019

References

[1] Vasconcelos D, Silva A, Barata J. Influence of Vapour Bubbles Size and Spacing on Droplet Impact Outcomes under Subcooled Boiling Regimes. ILASS–Europe 2022, 31st Conference on Liquid Atomization and Spray Systems.

[2] Popinet, S. Basilisk flow solver and PDE library. http://basilisk.fr.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Use of combined electromagnetic fields for improved welding process

Kaldre Imants*
* University of Latvia
Institute of Physics
Riga, Latvia
e-mail:imants.kaldre@lu.lv

Abstract: Welding is very important in numerous industries ranging from automotive and aviation to shipbuilding and pressure vessel production. For large plate welding, high heat input welding causes various problems related to rapid local overheating and the formation of inhomogeneous post-weld microstructure. Welding is also used in additive manufacturing, which is rapidly developing technologies nowadays. Since welding is a complex multiphysical process there are various parameters such as electric current, oxygen presence, slag composition, heat flow and weld pool flow which influence the quality of welding joint and efficiency of the process. In this work we experimentally and numerically investigate how to modify heat and mass transfer in weld pool and heat affected zone by applied electromagnetic fields. Electromagnetic field is one of the ways how to affect the molten metal flow by changing the electromagnetic force distribution in the weld pool. Experimental setup is developed for investigation of the controlled welding with applied magnetic fields and their combinations (AC field, DC field, pulsed field, gradient field). It is found that DC magnetic field has influence on joint morphology and microstructure.

Keywords: Welding, Electromagnetic field, Additive manufacturing, Magnetohydrodynamics

1. Introduction

During welding process of steel plates multiple physical processes take place. To connect thick plates with single weld high heat input welding is used and nowadays welding energy can be as high as 500 kJ/cm [1]. Heat and mass transfer in weld pool are largely influenced by electromagnetic forces, because of high current density. Melt flow in the weld pool have significant influence on heat transfer and impurity transport. These can be the key factors for weld joint material structure and quality [2]. Melt flow can be created by several different effects. Well described effects in welding are Marangoni convection due to surface tension-temperature dependence, buoyancy convection due to density temperature dependence and electro-vortical flow due to the weld current self-induced magnetic field interaction [3]. Previous research has been devoted to the study of the slag properties and various welding process parameters and their influence on the result [4-6]. It is shown that electro-vortical flow, Marangoni convection, natural convection are the main mechanisms driving liquid metal flow in the weld pool [7]. This is important because flow is closely linked to the temperature regime and heat transfer in the weld pool and local cooling rate [8]. Cooling rate is one of the main aspects, which determine the structure and properties of the solidified metal [9].

2. Results

Shipbuilding steel AH36 plate is welded under DC magnetic field of 0.07 T. Experiment is done in small scale using a regular welder and 3.2 mm rutile coated electrode (-). Weld current is 150 A in all experiments and welding velocity is 10 mm/s. Magnetic field is created by permanent magnet assembly, which can be turned to get all orientations of the magnetic field.

Experimental results are summarized in the Fig. 1, showing the cross sections with various magnetic field orientations. Reference experiment without DC magnetic field is shown in Fig. 1a, in this case joint and heat affected zone is symmetric. According to estimations we can assess the fluid flow direction in each case with DC magnetic field. If DC magnetic field is applied perpendicular to the welded plate than the Lorentz force acts on the molten weld pool and flow is induced to the one side of the joint as can be seen in Fig. 1b. In case of magnetic field along the joint direction shown in Fig. 1c force is also acting perpendicular to the joint

which can be seen as asymmetric joint and HAZ. If static magnetic field is applied perpendicular to the weld direction, then Lorentz force acts along the joint potentially leading to improved heat transfer in longitudinal direction along the joint direction Fig. 1d. Experimental results are in good agreement with numerical simulation results of the MHD flow in the weld pool.

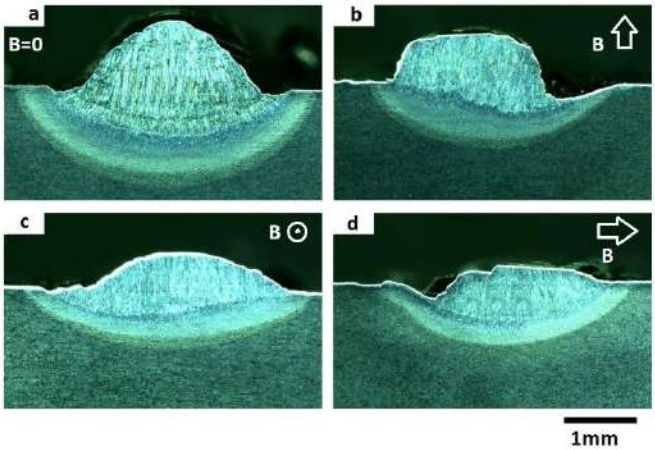


Figure 1. Cross section of the weld joint under different direction of static magnetic fields. Here I=150 A, u=1 cm/s, B=0.07 T: a) Reference experiment, b) Magnetic field from bottom, c) Magnetic field along welding direction, d) Magnetic field perpendicular to welding

4. Conclusions

This work experimentally demonstrates that static magnetic field could be used to affect the joint and heat affected zone morphology. Novadays more and more popular are combined welding processes which you use DC and AC current simultaneously. Application of external magnetic fields can potentially be another tool how to modify heat and mass transfer.

References

[1] P. Zhang, J. Zhang, B. Li, Mechanical Properties and Microstructure Transformation Behaviour for Welded Joints in Ship Plate Steel with High-Heat Input Welding, Journal of Material Engineering and Perform. 79(2021).

[2] M. Stadler et al, Experimental characterization of the weld pool flow in a TIG configuration. Journal of Physics: Conference Series. 550(2014), 012005.

[3] V. Bojarevics, J. Freibergs, E.I. Shilova, E.V. Shcherbinin. Electrically Induced Vortical Flows, Kluwer Academic Publishers, Dordrecht, Boston, London (1989)

[4] J. Zhang, T. Coetsee, H. Dong et.al, Element Transfer Behaviors of Fused CaF2-SiO2-MnO Fluxes Under High Heat Input Submerged Arc Welding. Metallurgical and Materials Transactions B. 51(2020) 885–890.

[5] J. Zhang, T. Coetsee, C. Wang. Element Transfer Behaviors of Fused CaF2-SiO2 Fluxes Subject to High Heat Input Submerged Arc Welding. Metallurgical and Materials Transactions B. 51(2020) 16–21.

[6] J. Zhang, T. Coetsee, H. Dong, et al. Elucidating the Roles of SiO2 and MnO upon Decarburization During Submerged Arc Welding: A Thermodynamic Study into EH36 Shipbuilding Steel. Metallurgical and Materials Transactions B. 51(2020)1805–1812.

[7] A. Kumar and T. DebRoy. Calculation of three-dimensional electromagnetic force field during arc welding. Journal of Applied Physics. 94(2003)1267.

[8] L. Aucott, H. Dong, W. Mirihanage, et al. Revealing internal flow behaviour in arc welding and additive manufacturing of metals. Nature Communications. 9(2018) 5414.

[9] L. Jae-Hyeong, Y. Shotaro, O. Tomo, S. Kazuyoshi, Effects of cooling rate on solidification cracking behaviour in 310S stainless steel. Journal of Advanced Joining Processes. 3(2021), 100044.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Constitutive Modelling and Validation of TRIP Steels

R. P. Cardoso Coelho*, M. Vieira de Carvalho*, F. M. Andrade Pires*

*Department of Mechanical Engineering (DEMec)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: ruicoelho@fe.up.pt, mvcarvalho@fe.up.pt, fpires@fe.up.pt

Abstract: The combination of high strength and ductility in steels has been pursued throughout the decades to fulfill industrial requirements. Among the so-called advanced high-strength steels, Transformation-Induced Plasticity (TRIP) alloys have gained particular traction over the last years due to the their reduced productions costs. The mechanically-induced transformation from retained austenite to martensite promotes a strain hardening effect that enhances the ductility of these materials. A finite-strain micromechanical single-crystal constitutive model accounting for irreversible martensitic transformations and crystallographic slip in both phases is formulated in this work. The non-unique solutions for linearly-dependent systems are addressed via a rate-dependent regularisation in a fully implicit return-mapping algorithm combining a volume-preserving exponential mapping integrator and a generalisation of Patel and Cohen's energy-based criterion for martensitic transformation. When embedded in a multi-scale finite element framework, the macroscopic response is derived from the computational homogenisation of Representative Volume Elements (RVEs). Compared with previous works [1,2], relevant terms are introduced in the thermodynamic driving forces to better recover the experimental response of these materials. The model is validated with available results in the literature [3] using an automated parameter identification tool. Finally, certain modelling simplifications are explored to reduce the number of local equations when martensite plasticity is admitted.

Keywords: Crystal Plasticity, Phase Transformation, FEM, Multi-scale Models

References

[1] Carvalho, Miguel Vieira de, Daniel de Bortoli, and Francisco M. Andrade Pires. 2022. Consistent Modeling of the Coupling between Crystallographic Slip and Martensitic Phase Transformation for Mechanically Induced Loadings'. International Journal for Numerical Methods in Engineering.

[2] Turteltaub, S., and A. S. J. Suiker. 2006. 'A Multiscale Thermomechanical Model for Cubic to Tetragonal Martensitic Phase Transformations'. International Journal of Solids and Structures 43 (14): 4509-45.

[3] Perdahcioğlu, E. S., and H. J. M. Geijselaers. 2012. 'A Macroscopic Model to Simulate the Mechanically Induced Martensitic Transformation in Metastable Austenitic Stainless Steels'. Acta Materialia 60 (11): 4409-19.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modeling technique for petiole-lamina connections of peltate leaves

Stephan Ritzert[1], Hagen Holthusen[1], Domen Macek[1], Annabell Rjosk[2], Thea Lautenschläger[2], Christoph Neinhuis[2] and Stefanie Reese[1]

[1] Institute of applied mechanics
RWTH Aachen University
Aachen, Germany

[2] Institute for Botany
Technische Universität Dresden
Dresden, Germany

Abstract: Peltate leaves, where the petiole is attached on the underside of the leaf blade, act as a model for novel lightweight carbon fiber reinforced structures. In petiole-lamina connections, the fibers (sclerenchyma) are redirected from the leaf blade (lamina) into the leaf stalk (petiole). Modeling these fiber bundles with the finite element method would require very fine meshes, to distinguish between matrix and fiber parts. In this work, we use only one mesh for both constituents and embed information about the fiber bundles. For every element, we compute the fiber content and the averaged fiber direction as internal variables. These quantities are integrated into a transversely isotropic viscoelastic material model for finite strains, where the fiber content of the element scales the anisotropic part. The fiber geometry is discretized as a point cloud with orientation vectors at every point. This data can be computed from segmented computer tomography data.

Keywords: Anisotropy, FEM, Viscoelasticity

1 Introduction

In this work, we present a method to simulate the petiole-lamina connections of peltate leaves, which are leaves where the petiole is attached to the underside of the leaf blade. The load is transferred by fiber bundles from the leaf blades into the petiole. Different peltate-leaved species show different fiber bundle structures and orientations in the transition zones. The load-bearing mechanisms of these plants should be analyzed to inspire new carbon fiber-reinforced constructions. The complex anatomy of these reinforcing structures makes creating a finite element model difficult. Therefore, we represent the fiber bundles with a vector field and superimpose this field with a finite element mesh. In the elements containing fibers, we use a transversely isotropic viscoelastic material model for finite strains. In all other elements, we use a finite strain, isotropic viscoelastic material model

2 Model

The fiber bundles are modeled by considering a transversely isotropic material only in elements containing fibers. For every element, we compute the fiber content

$$\alpha_F = \frac{k_p}{k_e}, \tag{1}$$

where k_p is the number of fiber points per element and k_e is the maximum number of points per element. Furthermore, we define the averaged fiber direction as

$$\boldsymbol{n}_F := \frac{1}{k_p} \sum_{p=1}^{k_p} \boldsymbol{n}_{F,p}. \tag{2}$$

The mechanical behavior of plant tissue is time-dependent. Therefore, we model both constituents by a viscoelastic material model. The model used here is a modification of the material model developed in Macek et al. [1]. This model is based on the multiplicative split of the deformation gradient into elastic and inelastic parts

$$\boldsymbol{F} = \boldsymbol{F}_e^{iso} \boldsymbol{F}_i^{iso} = \boldsymbol{F}_e^{ani} \boldsymbol{F}_i^{ani}. \tag{3}$$

Based on this split we define the right Cauchy-Green strain tensors for both constituents:

$$\boldsymbol{C} = \boldsymbol{F}^T \boldsymbol{F} \tag{4}$$

$$\boldsymbol{C}_e^{iso} = \boldsymbol{F}_e^{iso^T} \boldsymbol{F}_e^{iso}, \quad \boldsymbol{C}_i^{iso} = \boldsymbol{F}_i^{iso^T} \boldsymbol{F}_i^{iso} \tag{5}$$

$$\boldsymbol{C}_e^{ani} = \boldsymbol{F}_e^{ani^T} \boldsymbol{F}_e^{ani}, \quad \boldsymbol{C}_i^{ani} = \boldsymbol{F}_i^{ani^T} \boldsymbol{F}_i^{ani} \tag{6}$$

The anisotropy is accounted for by structural tensors, that are computed from the averaged fiber direction

$$\boldsymbol{M}_F = \kappa \, \boldsymbol{I} + (1 - 3\,\kappa)\, \boldsymbol{n}_F \otimes \boldsymbol{n}_F, \quad \bar{\boldsymbol{M}}_F = \frac{\boldsymbol{F}_i^{ani} \boldsymbol{M} \boldsymbol{F}_e^{ani^T}}{\boldsymbol{C}_i^{ani} \cdot \boldsymbol{M}} \tag{7}$$

where κ is the dispersion factor and $\bar{\boldsymbol{M}}$ is the structural tensor in the intermediate configuration. Based on these definitions, the Helmholtz free energy is

$$\psi = \psi_{eq}^{iso}(\boldsymbol{C}) + \psi_{neq}^{iso}(\boldsymbol{C}_e^{iso}) + \alpha_F \left(\psi_{eq}^{ani}(\boldsymbol{C}, \boldsymbol{M}) + \psi_{neq}^{ani}(\boldsymbol{C}_e^{ani}, \bar{\boldsymbol{M}}) \right). \tag{8}$$

Here the anisotropic contributions are scaled by the fiber content α_F (Eq. 1). Both isotropic and anisotropic parts have an equilibrium free energy accounting for the elastic response and a nonequilibrium part responsible for the viscoelastic response. The nonequilibrium parts depend on tensors in the intermediate configuration. For the definition of the free energy parts, evolution equations, and an explanation of the numerical implementation, the reader is referred to Macek et al. [1].

With this model different plants with different fiber paths can be computed with coarse meshes. It simplifies the modeling process since the fiber bundles do not have to be modeled explicitly. The vector field can either be computed from splines or from segmented CT Data.

3 Acknowledgements

Funding granted by the German Research Foundation (DFG) within the subproject A01 of the Transregional Collaborative Research Center (CRC) Transregio (TRR) 280 with project number 417002380 is gratefully acknowledged.

References

[1] Macek D, Holthusen H, Rjosk A, Ritzert S, Lautenschläger T, Neinhuis C, Reese S. Mechanical investigations of the peltate leaf of Stephania japonica (Menispermaceae): experiments and a continuum mechanical material model. Front. Plant Sci. 2023; 4139.

Prediction of crack evolution in TiN thin films deposited on different substrates based on cohesive elements

K. Perzynski[*], G. Cios†, L. Madej[*]

[*]Faculty of Metals Engineering and Industrial Computer Science,
AGH University of Science and Technology,
Krakow, Poland
e-mail: kperzyns@agh.edu.pl

[†]Academic Centre for Materials and Nanotechnology,
AGH University of Science and Technology,
Krakow, Poland
e-mail: gcios@agh.edu.pl

Abstract: This study presents a new approach to the numerical analysis of crack evolution in thin films made of titanium nitride (TiN) pulsed laser deposited (PLD) on the surface, taking into account the morphology of the thin film in an explicit manner. TiN thin films deposited on different substrates were selected as a case study for the research. The mechanical properties of the thin film and the substrates were determined with the nanoindentation tests conducted in laboratory conditions. Based on the performed tests and inverse analysis, the hardening curves for TiN and substrates were determined and then applied to the numerical modelling of crack formation under loading conditions. The plugin for Abaqus software was implemented to deliver a digital material representation model of the investigated thin film. The crack propagation model was developed within the finite element method considering the cohesive type elements. The obtained numerical results are validated against a series of experimental data. The study proved that the model based on the concept of digital material representation could be used for reliable predictions of local crack development in thin films deposited by the PLD method.

Keywords: pulsed laser deposition; thin films; digital material representation; inverse analysis; cohesive zone;

1. Introduction

Titanium nitride (TiN) thin films are widely used materials for obtaining products with a high degree of biocompatibility and high strength resistance at the same time (e.g., implants). Therefore, TiN films are used in implantology, from knee joint replacements to pump valves supporting the human heart [1]. However, transmission and scanning electron microscopy analysis revealed the frequent occurrence of a complex columnar nanostructure in these materials resulting from the specific nature of the Pulsed Laser Deposition (PLD) [2] process. The morphology of such nanostructure is one of the main reasons for uncontrolled delamination and fracture observed in thin films under loading conditions.

Accurate analysis of thin film cracking requires a series of very sophisticated laboratory experiments. These studies are often time-consuming and expensive. Therefore, as the capabilities of modern Computer Aided Engineering (CAE) applications significantly increased in recent years, they are frequently used to support experimental investigations. The possibilities offered by the modern Digital Material Representation (DMR) approaches have been explored in particular [3]. DMR can be treated as replicas of real microstructures for further numerical simulations. Such models allowtransferring of nanostructural behaviour responsible for the fractures and delamination process directly to the numerical simulation. Information on the local heterogeneities in the thin film morphology is crucial to investigate fracture initiation.

2. Numerical model of nanoindentation test

The work extends the mentioned DMR-based research and incorporates information on the heterogeneous morphology of the columns in the deposited film. The full-field model was developed based on quantitative transmission electron microscopy investigation. The cohesive zone elements were also introduced to determine critical values for fracture initiation and

delamination in TiN thin film deposited on different substrates, namely Si, Al, Steel, Cu. An example of obtained results is presented in Figure 1.

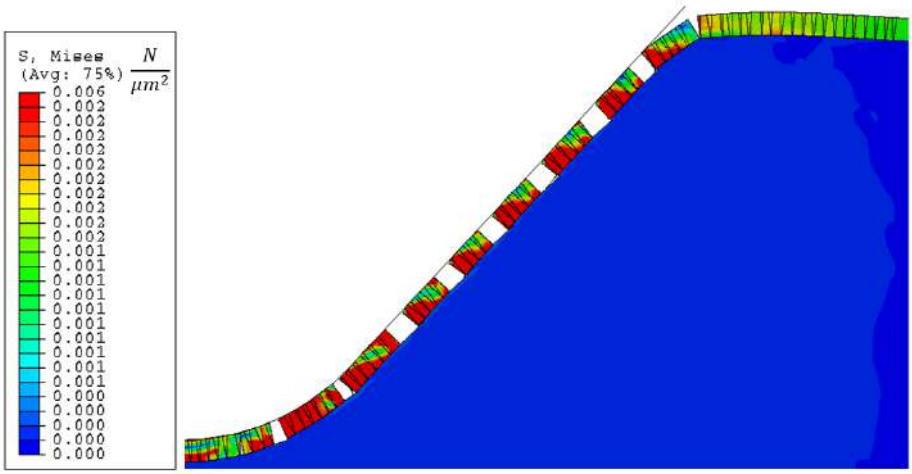


Figure 1. Stress distribution with fractures in TiN thin film deposited on Al after nanoindentation test.

To prove the predictive capabilities of the developed full-field model, the numerical results are validated against the laboratory nanoindentation data revealing the film behaviour under loading. It was also demonstrated that the approach could be directly used in commercial finite element software, which is important for wide application across the community.

Acknowledgements
Numerical calculations have been performed with the use of the PLGrid Infrastructure. The work was realized as a part of fundamental research financed by the Ministry of Science and Higher Education grant no. 16.16.110.663.

References
[1] A. Ahmed, X. Wang, and M. Yang, Biocompatible materials of pulsatile and rotary blood pumps: A brief review, Reviews On Advanced Materials Science 59; 1: 322–339, 2020.
[2] K. Perzynski, G. Cios, G. Szwachta, D. Zych, M. Setty, P. Bala, L. Madej, Numerical modelling of a compression test based on the 3D digital material representation of pulsed laser deposited TiN thin films, Thin Solid Films 673: 34–43, 2019.
[3] K. Perzynski, The effect of model size and boundary conditions on the representativeness of digital material representation simulations of ferritic-pearlitic sample compression, Computer Methods in Materials Science 22; 2: 59–66, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

The operator spectrum of linear elasticity least-squares finite elements methods

Linda Alzaben*, Fleurianne Bertrand † and Daniele Boffi*,††

* Department of Applied Mathematics and Computational Science (AMCS)
King Abdullah University of Science and Technology(KAUST)
Thuwal, Kingdom of Saudi Arabia
e-mail: linda.alzaben@kaust.edu.sa
e-mail: daniele.boffi@kaust.edu.sa

† Department of Electrical Engineering, Mathematics and Computer Science (EEMCS)
University of Twente
AE Enschede, The Netherlands
e-mail: f.bertrand@utwente.nl

†† Dipartimento di Matematica "F. Casorati"
Università degli Studi di Pavia
27100, Pavia, Italy

Abstract: We investigate the spectrum of operators arising from the discretization with least-squares finite elements method. Particularly, we look into the first order system least-squares (FOSLS) for linear elastic problems in its two and three-field formulations. In our study, the discretization with the least-square finite element approach gives rise to a non-symmetric discrete formulation, on the contrary to the Laplacian which has a symmetric discrete formulation. Hence, complex eigenvalues are expected. We give some numerical analysis on the two-field case, and present some numerical results for both formulations. We are mainly interested in the behavior as we move to the incompressible limit. Thus, we show the strong dependency on the Lamé parameters and the underlying mesh.

Keywords: eigenvalue problems, linear elasticity, least-squares finite elements

1 Introduction

The first-order partial differential system for linear elasticity is called stress-displacement formulation. This formulation is comprised of the constitutive and equilibrium equations. The constitutive equation gives the relation between stress and strain tensors. Although one can obtain a second order problem with pure displacement, this is not preferred when for example one is interested in the stress, which can be obtained by differentiating displacement. Thus, the approximation order of the stress degrades. Several methods have been developed for the approximations of linear elasticity. Mixed finite elements (MFE) leads to a saddle point problem and requires a stable combinations between finite element spaces which are limited. Unlike the MFE, the advantage of least-squares is that the resulting choice of finite element spaces is not subject to stability conditions with its resulting algebraic system being positive definite and robust in the incompressible limit for the source problem [**?**].

2 The problem and convergence

Looking at the two field formulation least-squares, we consider the following problem:
Let Ω be a polytopal domain in $\mathbb{R}^d$ $(d = 2, 3)$, the minimization of the functional corresponding to the source problem is given by:

$$\mathcal{F}(\underline{\boldsymbol{\tau}}, \mathbf{v}; \mathbf{f}) = ||\mathcal{A}\underline{\boldsymbol{\tau}} - \underline{\boldsymbol{\epsilon}}(\mathbf{v})||_0^2 + ||\mathbf{div}\underline{\boldsymbol{\tau}} + \mathbf{f}||_0^2, \tag{1}$$

and gives rise to the eigenvalue variational problem:
Find $(\omega, \mathbf{u}) \in \mathbb{R} \times H^1_{0,D}(\Omega)^d$ with $\mathbf{u} \neq 0$ such that for some $\underline{\boldsymbol{\sigma}} \in \underline{\boldsymbol{X}}_N$ we have

$$\begin{cases} (\mathcal{A}\underline{\boldsymbol{\sigma}}, \mathcal{A}\underline{\boldsymbol{\tau}}) + (\mathbf{div}\underline{\boldsymbol{\sigma}}, \mathbf{div}\underline{\boldsymbol{\tau}}) - (\mathcal{A}\underline{\boldsymbol{\tau}}, \underline{\boldsymbol{\epsilon}}(\mathbf{u})) = -\omega(\mathbf{u}, \mathbf{div}\underline{\boldsymbol{\tau}}) & \forall \underline{\boldsymbol{\tau}} \in \underline{\boldsymbol{X}}_N, \\ -(\mathcal{A}\underline{\boldsymbol{\sigma}}, \underline{\boldsymbol{\epsilon}}(\mathbf{v})) + (\underline{\boldsymbol{\epsilon}}(\mathbf{u}), \underline{\boldsymbol{\epsilon}}(\mathbf{v})) = \mathbf{0} & \forall \mathbf{v} \in H^1_{0,D}(\Omega)^d. \end{cases} \tag{2}$$

The continuous problem possess positive real eigenvalues, but the least-squares formulation is not symmetric which gives, when discretized, complex eigenvalues that are spread in the complex plane. Moreover, non symmetry comes from the right hand side that is also singular. We give a brief idea on how to solve such a system, what are the eigenvalues expected and how we make use of the so called Schur complement. Moving to convergence analysis, we investigate in depth the uniform convergence of the solution operator by verifying the dual problem and using it to bound the error of the eigensolution under the L^2 norm. We then discuss the rate of convergence [**?**]. Finally, we present some numerical results confirming our theory and study the behavior of the spectrom as the material becomes incompressible, that is, the Lamé parameter λ first being small (elastic solid material) and then getting larger as we move to incompressiblility for both the two and three field [**?**] [**?**].

References

[1] Cai, Z. and Starke, G., 2004. Least-squares methods for linear elasticity. SIAM Journal on Numerical Analysis, 42(2), pp.826–842.

[2] Alzaben, L., Bertrand, F. and Boffi, D., 2022. On the spectrum of an operator associated with least-squares finite elements for linear elasticity. Computational Methods in Applied Mathematics.

[3] Alzaben, L., Bertrand, F. and Boffi, D., 2022. On the spectrum of the finite element approximation of a three field formulation for linear elasticity. Examples and Counterexamples, 2, p.100076.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Tuning Frequency Analysis of Energy Harvesting on Railway Bridges Using a Stochastic Process

Cámara-Molina, J.C.*, Romero, A.*, Galvín, P.*, Moliner, E.† and Martínez-Rodrigo, M.D.†

* Escuela Técnica Superior de Ingeniería, Universidad de Sevilla
Camino de los Descubrimientos s/n, ES-41092, Sevilla, Spain

† Universitat Jaume I, Department of Mechanical Engineering and Construction
Avda. Sos Baynat s/n, ES-12071, Castellón, Spain

Abstract: In this paper, the authors investigate energy harvesting on railway bridges. The tuning frequency for energy harvesters is studied. A stochastic process is proposed to find the tuning frequency from the mechanical energy collected from train-induced bridge vibrations. An energy harvester prototype is designed with PAHT-CF15 substructure. Energy losses due to detuning are analysed. The proposed approach is validated for an in-service bridge in a High-Speed line. Finally, the performance of energy harvesting is evaluated from in situ experimental data measured by the authors. The results allow to know the energy harvested for several train passages.

Keywords: Energy harvesting, railway bridges, High-Speed train, Stochastic process, tuning procedure.

1 Introduction

An important problem of energy harvesting systems is associated with the fact that the performance of the energy production device is limited to a very narrow operating frequency band around its resonance frequency [1]. If the excitation frequency deviates slightly from the resonance condition, the output power is drastically reduced. The objective of this work is the estimation of the frequency to which a harvester system should be tuned to maximise the energy collected in railway bridges.

2 Tuning procedure

An experimental campaign was carried out to assess the energy harvesting performance in a railway bridge in July-September 2022. The bridge under study belongs to the HSL Madrid-Sevilla.

Vibration levels under operating conditions were used to estimate the tuning frequency from the mechanical energy following a stochastic process. The mechanical energy [2] was computed for harvesters with a damping ratio of 1%. The confidence intervals, standard deviation, and mean values of the energy were estimated from the shape and scale parameters of a gamma distribution over the frequency range. Figure 1 shows the computed results. It can be observed a predominant frequency around 8 Hz where energy reaches its greatest values. There are also significant values of the energy around 9.3 Hz, which is interesting to note. Peaks below 5 Hz have not been taken into account because they correspond to bogie passage frequencies.

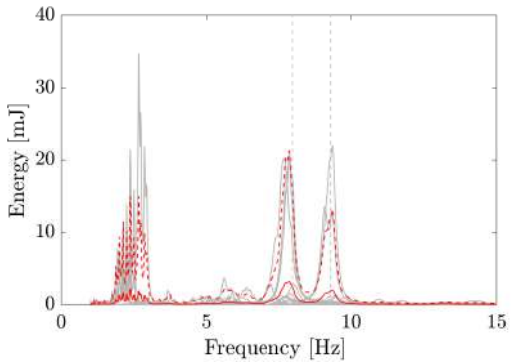


Figure 1: Mechanical energy from the bridge response for each train (solid grey lines), mean value (solid red line) and confidence interval (dashed red line).

The tuning frequencies (vertical dashed lines) were obtained from a normal distribution of the maximum peaks for each circulation around the frequencies 8 Hz and 9.3 Hz. The tuning frequencies $f_{t1} = 7.8\,\text{Hz}$ and $f_{t2} = 9.28\,\text{Hz}$ are obtained from the mean value of the normal distribution in both cases.

The estimated energy harvested by devices tuned to these frequencies are $E_{t1} = 9.173\,\text{mJ}$ and $E_{t2} = 6.380\,\text{mJ}$

3 Conclusions

The research presented here proposes a statistical procedure to estimate the tuning frequency of energy harvesters placed on railway bridges. The performance of harvesters for an in-service bridge on a High-Speed line has been analysed. The energy collected by harvesters tuned to the frequencies obtained from the statistical process has been estimated.

4 Acknowledgements

The authors would like to acknowledge the financial support provided by the Spanish Ministry of Science, Innovation and Universities under the research project PID2019-109622RB; PROYEXCEL_00659 funded by Junta de Andalucía (Regional Ministry of Economic Transformation, Industry, Knowledge and Universities); and the Andalusian Scientific Computing Centre (CICA).

References

[1] Erturk, A., & Inman, D.J., 2011, Broadband piezoelectric power generation on high-energy orbits of the bistable duffing oscillator with electromechanical coupling, Journal of Sound and Vibration, 330 (10): 2339–2353.

[2] Romero, A., Cámara-Molina, J.C., Moliner, E., Galvín, P. & Martínez-Rodrigo, M.D., 2021, Energy harvesting analysis in railway bridges: An approach based on modal decomposition, Mechanical Systems and Signal Processing, 160.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

An eXtended finite element method for the Nernst-Planck-Poisson equation

Pawan Kumar, Narasimhan Swaminathan, Sundararajan Natarajan*

Department of Mechanical Engineering, Indian Institute of Technology Madras
Chennai, 600036, India
*e-mail: snatarajan@smail.iitm.ac.in

Abstract: The Nernst-Planck-Poisson (NPP) set of equations is used to study the drifting mechanism in mixed ionic electronic conductors, commonly used in storage batteries. Depending on the size of the computational domain, the solution exhibits steep gradients near the boundaries, esp, in polycrystalline materials. As the grain boundary has different crystallographic orientations when compared to the bulk, to minimize the overall energy, charged defects redistribute between the grain boundary and the bulk grain. This redistribution introduces a steep gradient of ionic concentration and electric potential near the grain boundaries. Traditional finite element method, when employed requires extremely refined mesh to capture the steep gradient. To alleviate the meshing burden, in this work, we propose to augment the traditional finite element approximation space with a suitable ansatz to capture the steep gradient within the framework of the extended finite element method. The robustness and the accuracy of the proposed framework will be demonstrated by comparing with an overkill finite element solution. Later, the developed framework is employed to study the drifting mechanism in Lithium Lanthanum Titanium Oxide, a potential candidate for solid electrolyte material for lithium-ion batteries.

Keywords: eXtended finite element method, Nernst-Planck-Poisson equations, Solid electrolyte, Steep gradient

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Thermodynamically consistent Recurrent Neural Networks to predict non linear behaviours of dissipative materials subjected to non-proportional loading paths

Danoun Aymen[*,1], **Prulière Etienne** [2] **and Chemisky Yves**[1]

[1] Institute of mechanics and engineering (I2M)
Université de Bordeaux
Talence, France
e-mail: aymen.danoun1996@gmail.com, yves.chemisky@u-bordeaux.fr

[2] Institute of mechanics and engineering (I2M)
École Nationale Supérieure d'Arts et Métierso
Talence, France
e-mail: Etienne.PRULIERE@ENSAM.eu

Abstract: The present work aims at proposing an AI-based model using Thermodynamically Consistent Recurrent Neural Networks (ThC-RNN) to predict non-linear mechanical behaviors of dissipative materials under multi-axial and non-proportional loading paths. The development of such models can be a promising substitute for classical numerical methods for structural analysis (Finite Element Analysis, FFT methods) which often requires important computational costs. In fact, the new industrial constraints are nowadays pushing the limits of materials in terms of mechanical properties for advanced applications fields (energy, health, transport). The design of such structures can be limited by the numerical models capabilities when non-linear material behaviors occurs. The present work therefore proposes a new paradigm for the simulation of dissipative materials mechanical behavior by introducing a specific Neural Network architecture ThC-RNN. ThC-RNN proposed model present two major advantages over conventional Deep Learning ANN architectures as Multi-Layer Perceptrons (MLP). First, it is based on a specific RNN architecture called Stacked Long Short Term Memory (Stacked LSTM) which is adapted for solving path dependent problems. In that case, Neural Network output are not only related to the current input but also to the outputs of the past period of time through memory gates. The design of such architecture allows to take into account the loading history of dissipative materials subjected to complex loading paths (multi-axial and non-proportional loading paths). On the other hand, a special focus has been given to the respect of thermodynamics principles in the ThC-RNN model by introducing specific thermodynamical constraints during the training phase. Finally, the model's reliability has been tested on different plasticity models once the training is completed. Several mechanical quantities have been properly predicted by ThC-RNN model as stress tensor and tangent modulus components, state variables and mechanical works.

Keywords: Recurrent Neural Network (RNN), Plasticity, Dissipative materials, Non-proportional loadings paths, Thermodynamics

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modal identification of a portal frame railway bridge

J. Chordà-Monsonís[a,b], J.C. Sánchez-Quesada[b], A. Romero[a], E. Moliner[b], P. Galvín[a] and M.D. Martínez-Rodrigo[b]

[a] Escuela Técnica Superior de Ingeniería
Universidad de Sevilla, Camino de los Descubrimientos s/n, ES-41092
Sevilla, Spain
e-mail: chordaj@uji.es

[b] Department of Mechanical Engineering and Construction
Universitat Jaume I, Avda. Sos Baynat s/n, ES-12071
Castelló de la Plana, Spain

Abstract: In the design process of numerical models of railway bridges, it is usually necessary to update numerical models with experimental data. In the case of partially-buried structures such as portal frames, to obtain the modal parameters may lead to confusing results because of the co-existence of coupled modes with a high participation of the soil (soil modes from now on) and soil-structure modes, with a relevant deformation of the structure (structural modes) governing its response under operating conditions. In this work, the modal identification of a portal frame is carried out. The structural modes are identified based on experimental data and used to calibrate a 3D Finite Element numerical model of the portal frame with Perfectly Matched Layers as absorbing boundaries.

Keywords: Railway bridge, portal frame, modal analysis, experimental measurements.

1 Introduction

The dynamic response of portal frame bridges is substantially affected by Soil-Structure Interaction (SSI), which has a high associated computational cost. Because of this, SSI is usually neglected in the dynamic analyses [1]. Besides, the strong coupling between the soil and the structure complicates the obtention of experimental data useful to calibrate numerical models such as the bridge modal parameters. This work aims to: (i) identify the structural modes of an existing portal frame and then (ii) calibrate a 3D Finite Element (FE) numerical model of the bridge padded with Perfectly Matched Layers (PMLs) to avoid boundary reflections and reduce the computational cost.

2 Modal analysis of the portal frame

The portal frame under study is found on the High-Speed (HS) line Madrid-Sevilla at the kilometric point 31+200. Three tracks pass over the bridge: two for HS services and one for conventional traffic. The frame has 8 m of span length, 22.10 m width and 5.7 m height, and is divided into two structures by a longitudinal joint (purple dashed line in Fig. 1). A 3D FE model of the bridge is implemented with PMLs enclosing the soil domain. During the experimental campaign, 27 accelerometers, shown as red circles in Fig. 1, were installed. Acceleration data was recorded at a sampling frequency of 4096 Hz and decimated (order 16). A third-order Chebyshev filter with high-pass frequency of 1 Hz was applied.

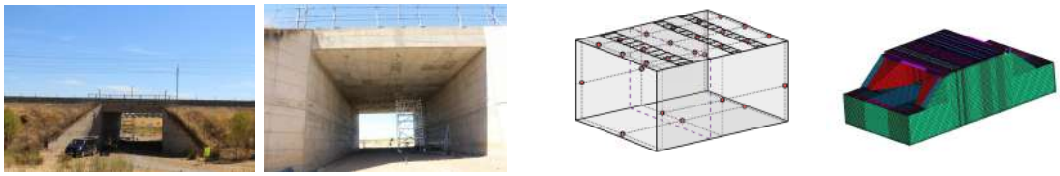


Figure 1: Two views of the bridge, accelerometers layout and numerical model.

First, an OMA is carried out from the ambient vibration of the structure using the Enhanced Frequency Domain Decomposition (EFDD) method. Due to the strong influence of the soil, it is difficult to distinguish between soil and structural modes. For this reason, the Frequency Response Functions (FRF) of 27 train passages in all sensors are also analysed. Clear frequency peaks detected with both approaches are found as modes with a predominant participation of the bridge structure. These modes are then used to calibrate the numerical model. Sufficient soil and PML lengths are used to ensure the stability of the solution. The PML layer surrounding the soil ensures the absortion of propagating waves and avoids spurious boundary reflections. A uniform homogeneous soil type is considered in a first approach. The calibration process is counducted based on a series of harmonic analyses while variying the mechanical properties of the soil and the bridge under acceptable ranges. Finally, after proper calibration, the first two natural modes of the bridge are replicated with the numerical model: f_1=26.8 Hz, ζ_1=0.48 % and f_2=44.3 Hz, ζ_2=0.55 %.

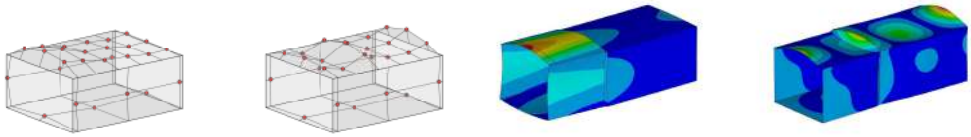


Figure 2: First two structural mode shapes. Left: OMA. Right: numerical model.

3 Conclusions

It can be concluded that, due the complexity induced by the influence of the soil, comparing the experimental data from an OMA and from several train passages may be a proper manner to identify the main structural modes of a portal frame. The results of the study are valid and the use of PMLs has allowed to reduce the computational cost of the procedure.

4 Acknowledgements

The authors acknowledge: Junta de Andalucía and ESF (USE-22311-R); Ministerio de Ciencia e Innovación (PID2019-109622RB-C2) and Generalitat Valenciana (AICO/2021/200).

References

[1] Zangeneh, A., François, S., Lombaert, G., Pacoste, C. Modal analysis of coupled soil-strcuture systems, J. of Soil Dynamics and Earthquake Engineering 2021;144;106645

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Railway induced vibrations in skewed double-track girder bridges

J.C. Sánchez-Quesada*, A. Romero†, P. Galvín†, E. Moliner * and M.D. Martínez Rodrigo*

* Department of Mechanical Engineering and Construction (MMCTE)
Universitat Jaume I
Castelló de la Plana, Spain
e-mail: jquesada@uji.es

†Escuela técnica superior de ingeniería
Universidad de Sevilla
Sevilla, Spain

Abstract: This work studies the dynamic performance of oblique railway bridges composed by SS spans, weakly connected through the ballast bed, and girder decks with end diaphragms. To do so, a detailed 3D model of an existing skewed bridge is developed and calibrated with experimental measurements. Then, a parametric analysis is performed to evaluate the folllowing three aspects: (i) deck obliquity, (ii) the presence of diaphragms at span ends and (iii) the influence of numerical modes different to the longitudinal bending one. Finally, a numerical-experimental comparison of the bridge response under a train passage is performed. Conclusions regarding the most relevant mode contributions in function of deck obliquity and the influence of diaphragms on the dynamic response are devised.

Keywords: Transverse Diaphragms, Skewness, Railway Bridges, Ballasted Track, Moving loads

1 Introduction

Railway bridges composed by simply-supported (SS) spans of short-to-medium length are critical in terms of train-induced vibrations, and thus, an accurate prediction of the vertical acceleration levels under traffic actions is essential. Many current standard methods rely on the premise that the response of SS railway bridges is dominated by the first longitudinal bending mode, and therefore, simplified beam models are accepted in preliminary steps of the design process. However, this may not be the case for double-track bridges with highly skewed decks. Preliminary studies about the influence of end diaphragms on the dynamic performace of oblique girder bridges have been performed [1], but most of the work found disregard the weak coupling exerted between successive spans through the ballast bed. A detailed 3D finite element (FE) model of an existing skewed double-track girder bridge with multiple SS spans, including an accurate representation of the ballasted track, is developed in this study to derive further conclusions about the adequacy of simplified beam models.

2 Methodology and results

Figure 1 shows the highly skewed (skew angle $\beta = 134°$) girder bridge under study and a detail of its FE model developed in ANSYS(R)17, which includes a continuous representation of the ballasted track and also the transverse diaphragms at each span end. The model is calibrated with a Genetic Algorithm, using the real modal parameters experimentally identified

from ambient vibration. A sensitivity analysis is next carried out to study the correlation of deck geometric characteristics (obliquity, presence/absence diaphragms) on its dynamic performance under forced vibration focusing on the predominant mode contributions. Also, an experimental-numerical comparison of the deck vertical acceleration under train passage is performed to evaluate the model accuracy. The numerical response is computed by mode superposition, considering moving loads for the vehicle.

Figure 1: From left to right: Lateral view of the bridge. Diaphragms details. Numerical model.

Figure 2 (a,b) shows the maximum acceleration response computed under HSLM-A train passage neglecting (a) and considering (b) the bridge skew angle and including a different number of mode contributions. Figure 2 (c,d) shows an experimental (black)-numerical comparison of the vertical acceleration response under a high-speed train passage considering (i) the skewed calibrated model (red) and (ii) the same model ignoring obliquity (grey).

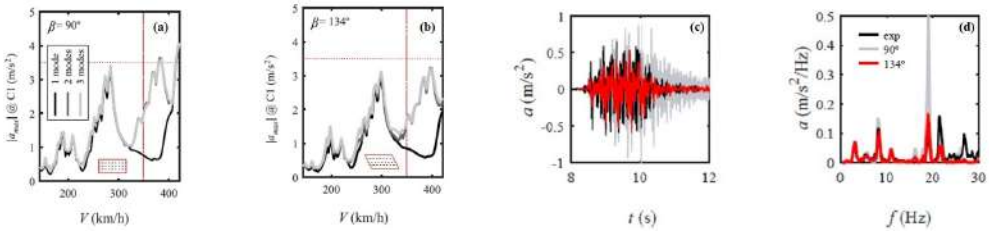


Figure 2: Modal contribution on straight and skew bridge (a-b). Numerical-experimental comparison (c-d).

3 Conclusions

The results show that the modelling simplifications admitted for straight decks may not be adequate for highly skewed bridges. For an accurate prediction of the vertical acceleration levels in these decks, a detailed modelling of the boundary conditions at span ends is relevant as well as to account for mode contributions different from the longitudinal bending. Also, the overall maximum acceleration under train passage reduces with the deck obliqueness.

4 Acknowledgements

Ministerio de Ciencia e Innovación (PID2019-109622RB-C2); Generalitat Valenciana (AICO/2021/200); Univ. Jaume I (UJI-B2021-16).

References

[1] Moliner E, Romero A, Galvín P, Martínez-Rodrigo M.D. Effect of the end cross beams on the railway induced vibrations of short girder bridges. Eng Struct 2019;201:109728.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Catenary design by sequential parameter optimisation

Gil Jaime[*], Gregori Santiago[*], Tur Manuel[*] and Fuenmayor F. Javier[*]

[*] Institute of Mechanical and Biomechanical Engineering
Universitat Politècnica de València,
Valencia, Spain
e-mail: jaigiro@upv.es

Abstract: The optimisation of the pantograph-catenary interaction is addressed in this work, specifically, the geometrical optimisation of a catenary section with variable-length spans. This feature multiplies the number of optimisation parameters and makes conventional optimisation unattainable with reasonable computational cost. This problem has been solved by dividing the optimisation problem into multiple suboptimisations in which only two geometrical parameters are optimised. The suboptimisations are performed sequentially (going through the complete set of parameters) and iteratively (repeating the process for convergence of the optimum), leading to a very high reduction of the standard deviation of the pantograph catenary interaction force.

Keywords: pantograph, catenary, optimisation, interaction

1. Introduction

The catenary is the system responsible for providing energy to railway vehicles. The catenary design optimisation problem has been addressed by many authors [1]. The objective is to improve the mechanical behaviour of the catenary and the quality of the current collection. The availability of accurate simulation tools is essential for the feasibility and validity of such optimisations, thus, simulations of the pantograph-catenary interaction should fulfil the European Standard EN-50318.

The aim of this work is to illustrate a method of optimising the catenary geometry, i.e. dropper position and length of full sections of realistic catenaries, in which variable-length spans are found. Most of the catenary optimisations assume periodic spans [1], therefore, a small number of parameters are optimised due to this condition. In this work, the topology of every span is optimised, leading to a great number of parameters and a strategy is stated to perform the optimisation avoiding the inclusion of all parameters at once, which is not feasible due to the prohibitive computational cost.

2. Pantograph-Catenary sequential optimisation

The first requirement to perform a catenary optimisation is to be able to simulate the pantograph-catenary dynamic interaction. In this work, the catenary and pantograph models are developed according to [2]. The optimisation process consists of creating different candidates by means of an optimisation algorithm and evaluating the objective function for every candidate until the best is found. Every candidate is defined with the optimization parameter set. In this case, it includes the length and position of all the droppers of a catenary section. For each candidate, the simulated contact force is used to evaluate the performance, specifically, the standard deviation of the 20-Hz-low-pass filtered contact force is selected as the objective function to optimise.

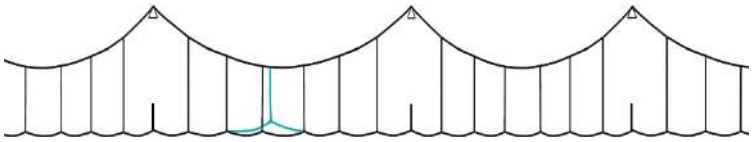


Figure 1. Catenary representation with the variation of the length and position of one dropper.

In a conventional use of an optimisation algorithm, all the parameters are included at once in order to attain the best solution. However, for this problem, the number of parameters is too high (more than a hundred per section) to optimise all of them at the same time. The solution adopted is to divide the optimisation into several suboptimisations, in which one-dropper parameters are optimised independently. Every suboptimisation is done sequentially, optimising every dropper from left to right (in the train running direction) and updating the catenary with the previous optimal solution. In Fig. 1, a catenary is depicted with a new candidate created by modifying the parameters of only one dropper. After optimising all droppers (a complete iteration), the process is repeated again but starting from the optimised catenary of the previous iteration. The Bayesian algorithm is used for every suboptimisation.

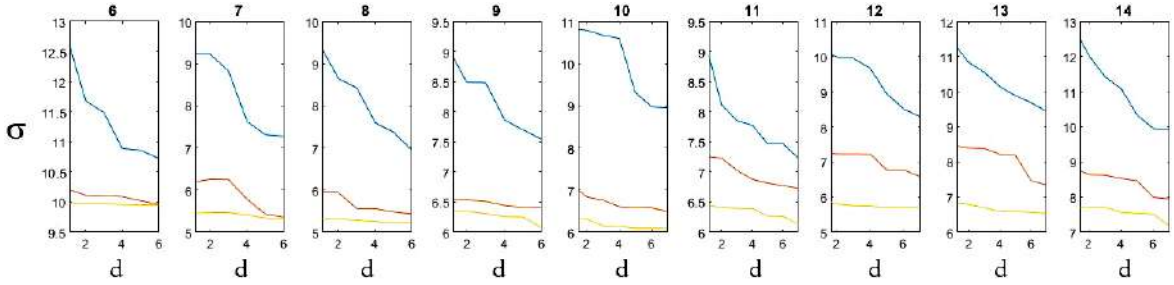


Figure 2. Standard deviation σ of the contact force (20 Hz filtered) of spans 6 to 14 after optimising dropper number *d* of the same span. The first, second and third iterations are in blue, orange and yellow, respectively.

The objective function of every suboptimisation is the standard deviation σ of the filtered contact force from 25 m before and after the span to which the optimising dropper belongs (in order to consider the influence of the dropper parameters). In Fig. 2, the objective function after optimising every dropper *d* of different spans (from 6 to 14) is represented for 3 iterations. In the graph, improvement is observed after every suboptimisation (respect *d*) and the improvement is present in every iteration but with less strength (the yellow curve is the flattest). This shows that the iterative process is converging to a solution. The optimisation has led to a reduction of the SMR of the contact force of 45%.

Acknowledgements

State Research Agency of the Spanish Science and Innovation Ministry (PID2020-113458RB-I00) and from the Valencian Regional Government (PROMETEO/2021/046)

References

[1] S. Gregori, M. Tur, E. Nadal, and F. J. Fuenmayor, An approach to geometric optimisation of railway catenaries, Vehicle System Dynamics, vol. 56, no. 8, pp. 1162–1186, 2018.

[2] S. Gregori, M. Tur, E. Nadal, J. Aguado, F. Fuenmayor, and F. Chinesta, Fast simulation of the pantograph–catenary dynamic interaction, Finite Elements in Analysis and Design, vol. 129, pp. 1 – 13, 2017.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Railway catenary shape-finding problem considering cantilevers and general track paths

Aldaz Nelson*, Gregori Santiago*, Gil Jaime*, Tur Manuel* and Fuenmayor F. Javier*

* Institute of Mechanical and Biomechanical Engineering
Universitat Politècnica de València,
Valencia, Spain
e-mail: nhaldsac@upvnet.upv.es

Abstract: In this article we propose a method to obtain the initial configuration of a railway catenary finite element model. To enhance the reliability of the catenary model, we propose to consider general track paths and cantilevers that support the cabling. The shape-finding problem is first solved for the cabling and then the cantilever of each support is independently considered by using conventional Euler beam elements. With the proposed approach, the number of degrees of freedom of the whole problem is reduced and thus, so is the computational cost. Additionally, the intricacy of setting displacement constraints in local coordinates is avoided.

Keywords: Railway catenary, shape-finding problem, cantilevers, general track paths.

1. Introduction

The interaction force between the railway catenary and the pantograph highly determines the current collection performance of the rail vehicles. Due to the high costs associated with the pantograph-catenary contact force measurement, in recent years several numerical models [1] have been proposed to simulate this dynamic interaction problem.

The first step to perform such a dynamic simulation is to solve the shape-finding problem of the catenary cabling. This work is aimed to propose an efficient procedure to compute the initial configuration problem of a catenary with considering realistic features such as general track layouts [2] and cantilevers on the supports.

2. Initial configuration problem

To model the catenary we use a finite element model based on the Absolute Nodal Coordinates Formulation (ANCF). The initial configuration is a non-linear problem in which the elements experiment large deformations. Following the idea proposed in [3], this problem consists on fulfilling both force equilibrium equations and design constraints (wire tension, contact wire height, dropper position, …), resulting in the system of equations (1), whose unknows are the nodal degrees of freedom $\boldsymbol{q}$ and the lengths of the undeformed elements $\boldsymbol{l}_0$.

$$\begin{aligned} F(\boldsymbol{q}, \boldsymbol{l}_0) &= 0 \\ C(\boldsymbol{q}, \boldsymbol{l}_0) &= 0 \end{aligned} \tag{1}$$

3. Methodology

To obtain the initial configuration of the catenary, we propose a substructuring approach divided into three steps.

- The first step consists on solving the initial configuration problem of the catenary cabling (Eq. (1)) in which the displacements of the connection points of the messenger wire with brackets and the contact wire with steady arms are fully constrained. These points are highlighted in black in Figure 1(a).

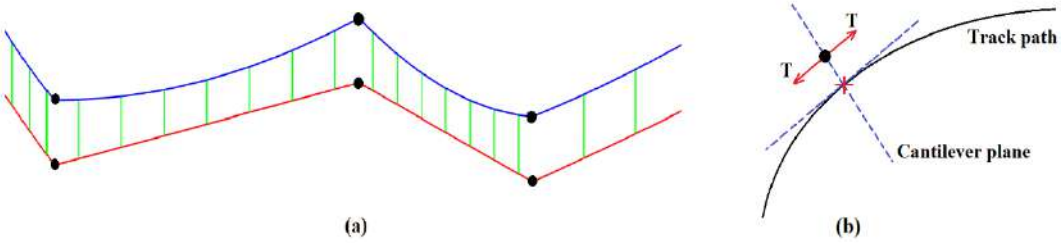


Figure 1. Additional constraints in the catenary supports.

  Additionally, the force of the wire in a perpendicular direction of the cantilever plane must be constant as depicted in Figure 1(b) to avoid rotation of the cantilever (when assembled in the last step). The reaction forces at these constrained points are also obtained.

- The design of each cantilever is carried out separately using as inputs the reaction forces obtained at the constrained points in the previous step. We propose to use conventional Euler beam elements to solve these 2D non-linear problems.
- Finally, the total structure is assembled by adding the cabling and all the cantilevers.

4. Conclusions

This work proposes a procedure to obtaine enhanced catenary models with general track paths and cantilevers. Solving the initial configuration of cantilevers separately presents two main advantages: avoid imposing constraints on local coordinates, thus eliminating the cumbersome coordinate transformation, and a decrease of the total degrees of freedom used, which entails a reduction in computational cost.

Acknowledgements

State Research Agency of the Spanish Science and Innovation Ministry (PID2020-113458RB-I00) and Valencian Regional Government (PROMETEO/2021/046).

References

[1] S. Bruni, J. Ambrosio, A. Carnicero, Y.H. Cho, L. Finner, M. Ikeda, S.Y. Kwon, J.-P. Massat, S. Stichel, M. Tur, The results of the pantograph–catenary interaction benchmark, Veh. Syst. Dyn. 2015;53 (3):412-435.

[2] Antunes, P., Ambrósio, J., Pombo, J., & Facchinetti, A, A new methodology to study the pantograph-catenary dynamics in curved railway tracks. Veh. Syst. Dyn. 2020;58 (3):425-452.

[3] M. Tur, E. García, L. Baeza, F.J. Fuenmayor, A 3D absolute nodal coordinate finite element model to compute the initial configuration of a railway catenary, Eng. Struct. 2014;71:234-243.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Computation of radiated noise from railway systems using a BEM-based procedure

Velázquez-Mata, R., Romero, A. and Galvín, P.

Escuela Técnica Superior de Ingeniería, Universidad de Sevilla
Camino de los Descubrimientos s/n, ES-41092, Sevilla, Spain
e-mail: rvmata@us.es

Abstract: This work studies vibration and radiated noise from railway systems using the 2.5D Boundary Element Method (BEM) formulation in the Bézier-Bernstein space. The proposed method allows the representation of the exact geometry of the track as it is done in computer-aided design (CAD) models. Thus, it is possible to evaluate problems with complex geometries, which are usually not adequately represented by the standard BEM and FEM formulations. Radiated noise is computed from the normal displacement at the boundary of the rail system according to the integral representation of the sound pressure. Only the track boundary is meshed, as the radiation condition is implicitly satisfied in the BEM fundamental solution. Moreover, the methodology allows the use of arbitrary high-order elements, making it efficient for the computation of radiated noise at high frequencies. The computed results are compared with some proposed by other authors.

Keywords: Radiated noise, Railway vibration, Boundary element method, Bézier curve

1 Introduction

The environmental noise from railways traffic is mainly due to the vibrations induced on the wheel and the track by the roughness of the running surfaces. Although both components of noise are significant, the radiated noise from the rail is often the highest, particularly for lower running speeds. Thus, it is important to improve the prediction capacities of the existing numerical models in order to compute the sound radiation from the different track systems, with the aim of mitigating its effects.

This works proposes a method that uses the 2.5D BEM formulation in the Bézier–Bernstein space to calculate vibration and radiated noise due to railways traffic. Therefore, it avoids mesh errors and enables evaluating the exact boundary geometry of complex rails profiles. This formulation also allows the use of arbitrary high-order elements, making it efficient for the computation of radiated noise at high frequencies.

2 Model and mobility for an open rail section

A standard CEN 40E1 rail profile and a pad with a thickness of $0.02\,\mathrm{m}$ were considered to validate the method. Figure 2 shows the 'point' mobility defined as the velocity at $x = 0$ divided by the force, for an excitation applied at the center of the rail-head as shown in Figure 1. This model was solved for a range of frequencies from 30 to $3500\,\mathrm{Hz}$. It can be seen a peak around $240\,\mathrm{Hz}$ due to the resonance of the rail mass on the stiffness of the rail pad.

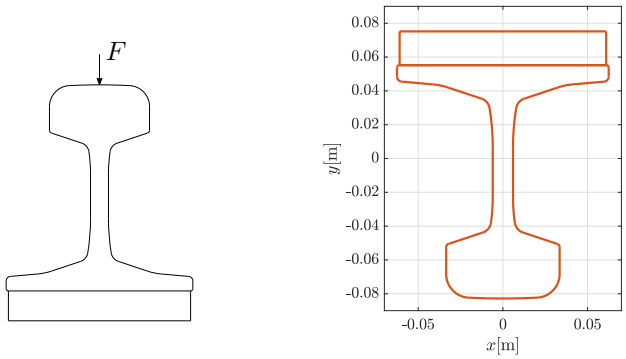


Figure 1: Force position and model of the rail CEN 40E1 and pad.

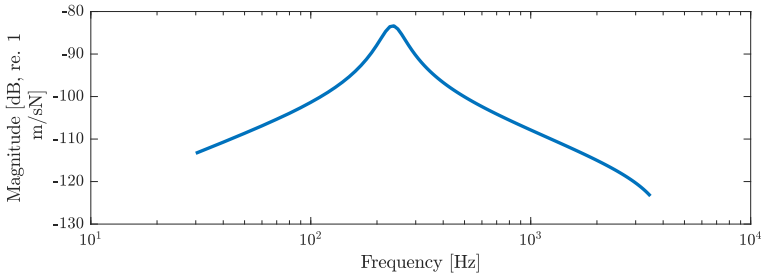


Figure 2: Point mobility of the open rail.

3 Conclusions

A BEM-based procedure to calculate the radiated noise from rails is proposed in this work. The possibility of implementing the exact geometry allows the evaluation of complex track systems concerning slab track and urban rail systems. Thus, the influence of track flexibility levels is studied. This methodology is also efficient for the computation of radiated noise at high frequencies, since arbitrary high-order elements can be used.

4 Acknowledgements

The authors would like to acknowledge the financial support provided by the Spanish Ministry of Science and Innovation under the research project PID2019-109622RB-C21, and US-126491 funded by the FEDER Andalucía 2014–2020 Operational Program. The support of the Andalusian Scientific Computing Centre (CICA) is gratefully acknowledged.

References

[1] Nilsson CM, Jones CJC, Thompson DJ, Ryue J. A waveguide finite element and boundary element approach to calculating the sound radiated by railway and tram rails. Journal of Sound and Vibration. 2009;321(3):813-36.

[2] Romero A, Galvín P, Cámara-Molina JC, Tadeu A. On the formulation of a BEM in the Bézier–Bernstein space for the solution of Helmholtz equation. Applied Mathematical Modelling. 2019;74:301-19.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Experimental characterization of a low-height acoustic barrier developed with numeric techniques

João Lázaro*, Pedro Alves Costa and * and Luís Godinho†

* CONSTRUCT
Faculty of Engineering (FEUP), University of Porto
Porto, Portugal

† ISISE
Department of Civil Engineering, University of Coimbra
Coimbra, Portugal;

Abstract: The increasing use of railway for transporting people and goods is essential to achieve a more environmentally and economically sustainable type of mobility. However, issues related to noise pollution caused by train traffic need to be mitigated so that there is a healthy coexistence between inhabitants and trains. This paper presents the experimental characterisation of a low height acoustic barrier to be used in railway environment, numerically developed in a first phase.

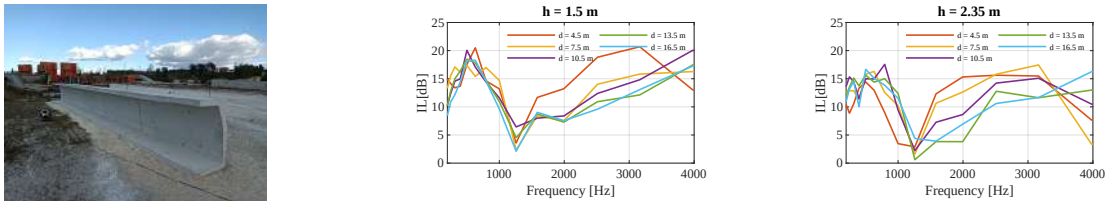
Keywords: Railway noise, Low heigh acoustic barriers, Experimental caracterization

1 Introduction

The railway system is the most sustainable mode of transport, with the lowest energy consumption. However, there is a severe problem related to high noise levels [5, 4]. Regarding mitigation, it widely used acoustic barriers. Although they guarantee a significant reduction of noise, their height is in itself a problem. Therefore, the use of low height acoustic barriers is a solution with proven efficiency [1, 2].

2 Tests and results

Firstly, tests were developed in free field, in order to have a global perception of the barrier's behaviour. As can be seen (Figure 1), the barrier offers a very satisfactory level of insertion loss for its height. It should be noted that the efficiency of the barrier largely depends on its use in a railway scenario [3, 6]

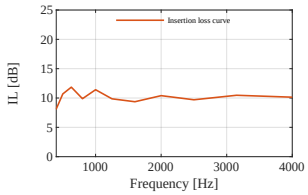


(a) (b) (c)

Figure 1: Measurement setup and results of Insertion loss for different microphone positions.

In a second phase, tests were carried out in a railway environment. The results obtained are quite satisfactory with relatively high levels of Insertion loss (Figure 2). The barriers were placed at approximately 1.60 m from the rail, and there is an increase in the efficiency of the barrier due to the constraints of the railway context for which the barriers were created [3, 6].

(a)



(b)

Figure 2: Setup of measurement and result of Insertion loss in railway environment

3 Conclusions

Noise mitigation along railway tracks is essential if the use of railways as a preferred means of transporting people and goods is to become an increasingly present reality. In the presented work, it was proved that this objective can be achieved with the use of acoustic barriers with optimised geometries.

References

[1] Koussa, F.; Defrance, J.; Jean, P.; Blanc-Benon, P. Acoustic performance of gabions noise barriers: numerical and experimental approaches. *Appl. Acoust.* **2013**, *74*, 189–197.

[2] Jolibois, A.; Defrance, J.; Koreneff, H.; Jean, P.; Duhamel, D.; Sparrow, V.W. In situ measurement of the acoustic performance of a full scale tramway low height noise barrier prototype. *Appl. Acoust.* **2015**, *94*, 57–68.

[3] Lázaro, João and Pereira, Matheus and Costa, Pedro Alves and Godinho, Luís Performance of Low-Height Railway Noise Barriers with Porous Materials *Applied Sciences* **2022**, *12*.

[4] EEA (European Environment Agency). Environmental Noise in Europe—2020; Technical Report; EEA (European Environment Agency): Copenhagen, Denmark, ISBN9789294802057.

[5] Blanes, N.; Marin, A.; Ramos, U.M.J. Noise Exposure Scenarios in 2020 and 2030 Outlooks for EU 28; European Topic Centre on Air pollution, transport, noise and industrial pollution – Norwegian Institute for Air Research: Kjeller, Norway, 2019.

[6] Lázaro, João and Pereira, Matheus and Costa, Pedro Alves and Godinho, Luís Numerical Development of a Low Height Acoustic Barrier for Railway Noise Mitigation; Recent Trends in Wave Mechanics and Vibrations: Proceedings of WMVC 2022; Lisboa, Portugal, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Experimental validation of the Hybrid Methodology for induced vibrations assessment

Soares, Paulo J.[1], Alves Costa, Pedro[1], Arcos, Robert[2] and Godinho, Lúis[3]

[1] Construct-FEUP
Faculty of Engineering, University of Porto
Porto, Portugal
e-mail: up201305102@fe.up.pt, pmbcosta@reit.up.pt

[2] Acoustical and Mechanical Engineering Laboratory (LEAM)
Universitat Politècnica de Catalunya (UPC)
Terrassa (Barcelona), Spain
e-mail: robert.arcos@upc.edu

[3] Department of Civil Engineering
University of Coimbra
Coimbra, Portugal
e-mail: lgodinho@dec.uc.pt

Abstract: In this work, an experimental validation of the hybrid methodology for the assessment of induced vibrations is presented. This methodology main advantage is the use of measurements as an input parameter, simplifying the usual numerical procedure, as it is no longer necessary to modulate the whole domain from the excitation source to the receiver, saving computational resources. It is determined a set of virtual forces, that when applied to the soil model induced the same displacement field on the location of the measurements. The application of these virtual forces to a soil-structure model will give the vibrations to which the structure will be subjected when will be constructed on that site. This methodology is validated experimentally on the Carregado experimental site.

Keywords: Hybrid Methodology, Induced Vibrations, Experimental

1 Introduction

Vibrations induced in structures by human activities have become a critical issue in urban areas, since new buildings are built in ever closer proximity to railway lines in operation. This phenomenon has led to the escalation of the problem of railway induced vibrations in buildings. For this, it is necessary to have a better understanding of the phenomenon, requiring the development of new tools and methodologies to study it. New approaches have been developed, the hybrid method for vibration prediction, proposed by Arcos et al.[1] and Costa et al.[2] is an innovative approach for the analysis of induced vibrations, which is based on the combination of field measurements with numerical simulations. This new proposal combines computational efficiency with uncertainty reduction in the predicted final value since it uses real on-site measurements as an input parameter of the methodology. The main objective of this work is to validate the hybrid methodology for the assessment of induced vibrations, on the experimental site of Carregado (Portugal).

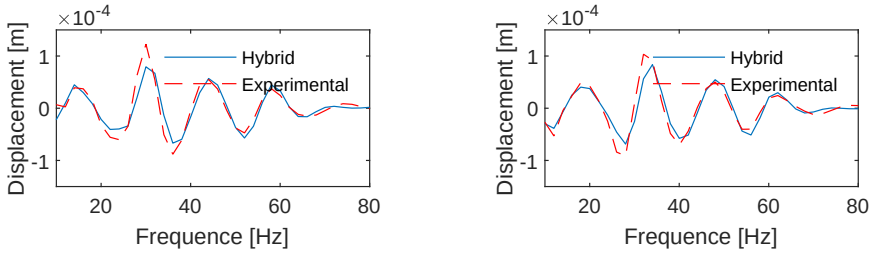


Figure 1: Comparison between the vertical response determined with the hybrid method and that measured experimentally: a) Real Part, b) Imaginary Part.

2 Hybrid methodology

This methodology combines measurements and numerical simulations, in order to obtain the vibration levels to which a structure will be subjected when built on the site where the experimental measurements were carried out.

The hybrid methodology consists on the determination of a set of virtual forces, which applied to a soil model generate an incident vibration field equal to the one measured experimentally. The application of the virtual forces to a soil-structure model allows obtain the vibrations in the structure induced by the experimentally measured wave field.

The hybrid methodology requires three steps: Step 1: Insitu measurements, at the collocation points; Step 2: Determination of the virtual forces; Step 3: Application of the virtual forces to a soil-structure model.

3 Experimental campaign

A set of experimental measurements were carried out in the already-known experimental field of Carregado. Consisted on the triaxial measurement of the vibration field induced at the 4 collocation points due to the application of an excitation, impact, at the ground surface, 6 meters from those points. The response measured at the accelerometers was processed and analyzed.

New tests were carried out at the evaluation points after the construction of the structure, a direct surface foundation (1x1x0.25 m). These measurements will be used to verify the accuracy of the hybrid method.

4 Validation

The hybrid method was applied, taking as input the experimental measurements made at the placement points. For both numerical models, soil and soil-structure, a semi-analytical method based on the Thomson-Haskell [3, 4] transfer matrix with the stabilization technique proposed by Wang [5]. The vertical response at the foundation obtained with the hybrid methodology was compared with the curve obtained experimentally, represented in Figure 1.

The agreement of the curves obtained allows the conclusion that the method presented can predict with high accuracy the induced vibration levels in a structure.

5 Conclusions

This paper presented the experimental validation of the hybrid methodology for the assessment of induced vibrations. This methodology main advantage is the use of measurements as an input parameter, simplifying the usual numerical procedure, as it is no longer necessary to modulate the whole domain from the excitation source to the receiver, saving computational resources.

The results of the validation show that the hybrid methodology can be used to accurately predict the vibration levels of a structure when it is built on a site with unknown soil characteristics and induced vibration field. The validation of the hybrid methodology on the experimental site in Carregado was successful, with the numerical simulations accurately predicting the field measurements.

References

[1] Arcos, R., Soares, P. J., Costa, P. A., Godinho, L. (2021). An experimental/numerical hybrid methodology for the prediction of railway-induced ground-borne vibration on buildings to be constructed close to existing railway infrastructures: Numerical validation and parametric study. Soil Dynamics and Earthquake Engineering, 150, 106888.

[2] P.A. Costa, R. Arcos, P. Soares, A. Colaço (2019). Hybrid approach for the assessment of vibrations and re-radiated noise in buildings due to railway traffic: concept and preliminary validation Advances in engineering materials, structures and systems: innovations, mechanics and applications - proceedings of the 7th international conference on structural engineering, Mechanics and Computation, pp. 79-84 2019.

[3] W.T. Thomson, Transmission of elastic waves through a stratified solid medium, Journal of Applied Physics. 21 (1950) 89–93.

[4] N.A. Haskell, The dispersion of surface waves on multilayered media, Bulletin of the Seismological Society of America. 43 (1953) 17–43.

[5] R. Wang, A simple orthonormalization method for stable and efficient computation of Green's functions, Bulletin of the Seismological Society of America. 89 (1999) 733–741.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Model order reduction for stochastic eigenvalue problems

Zhibao Zheng and Udo Nackenhorst

Institute of Mechanics and Computational Mechanics & International Research Training Group 2657
Leibniz Universität Hannover, Germany
e-mail: {zhibao.zheng, nackenhorst}@ibnm.uni-hannover.de

Abstract: This paper presents an efficient reduced-order method for stochastic eigenvalue analysis. In this method, stochastic eigenvectors are expanded into a sum of the products of unknown random variables and deterministic vectors, where deterministic vectors are calculated via a few deterministic eigenequations. Random variables and stochastic eigenvalues are solved by a reduced-order stochastic eigenvalue problem built by deterministic vectors. An example demonstrates the good accuracy of the proposed method.

Keywords: Model order reduction, Stochastic eigenvalue analysis, Reduced basis

1 Introduction

Stochastic eigenequations play important roles in stochastic dynamics analysis. However, existing numerical methods are expensive or computationally complex to solve this problem, e.g. the Monte Carlo simulation (MCS) [1] and the polynomial chaos-based method [2], etc. To this end, an efficient reduced-order method is presented in this paper.

2 Reduced-order method for stochastic eigenvalue analysis

In this paper, we consider the following stochastic eigenequation

$$\mathbf{K}(\theta)\,\mathbf{u}(\theta) = \lambda(\theta)\,\mathbf{u}(\theta), \tag{1}$$

where the stochastic matrix $\mathbf{K}(\theta) \in \mathbb{R}^{n\times n}$, $\mathbf{u}(\theta) \in \mathbb{R}^n$ and $\lambda(\theta)$ are stochastic eigenvectors and stochastic eigenvalues, respectively, n is the number of degrees of freedom. To solve Eq. (1), the m-th stochastic eigenvector is expanded via the following k-term approximation

$$\mathbf{u}_m(\theta) = \sum\nolimits_{i=1}^{k} \phi_m^{(i)}(\theta)\,\mathbf{d}_i = \mathbf{D}\boldsymbol{\phi}_m(\theta), \quad \mathbf{D} = [\mathbf{d}_i] \in \mathbb{R}^{n\times k},\ \boldsymbol{\phi}_m(\theta) = \left[\phi_m^{(i)}\right]^{\mathrm{T}} \in \mathbb{R}^k, \tag{2}$$

where $\phi_m^{(i)} \in \mathbb{R}$ are random variables and $\mathbf{d}_i \in \mathbb{R}^n$ are deterministic vectors. We introduce the stochastic residual $\mathbf{r}(\theta) = [\mathbf{K}(\theta) - \lambda(\theta)\,\mathbf{I}_n]\,\mathbf{d} \in \mathbb{R}^n$, which is minimized to solve the vector $\mathbf{d}_i$. The minimization $\min\limits_{\lambda(\theta)\in\mathbb{R},\mathbf{d}\in\mathbb{R}^n} \|\mathbf{r}(\theta)\|^2$ is equivalent to the following iteration [3],

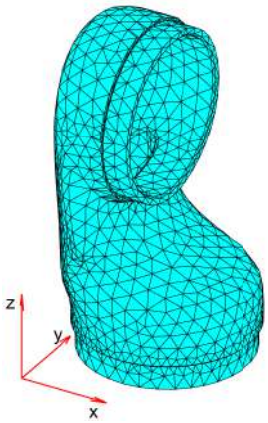
$$\mathbb{E}\{\lambda(\theta)\,\mathbf{K}(\theta)\} = \mathbb{E}\{\lambda^2(\theta)\}\mathbf{d}, \quad \lambda(\theta) = \mathbf{d}^{\mathrm{T}}\mathbf{K}(\theta)\,\mathbf{d}, \tag{3}$$

where the first equation is obtained by applying stochastic Galerkin procedure to $\mathbf{r}(\theta)$ under the known $\lambda(\theta)$ and used to solve $\mathbf{d}$ by deterministic eigenequations solvers, and the second equation is obtained by applying classical Galerkin procedure to $\mathbf{r}(\theta)$ under the known $\mathbf{d}$ and used to solve $\lambda(\theta)$. The final solution of $\mathbf{d}$ is obtained by repeatedly solving Eq. (3). A similar iteration is used to calculate other vectors and the Gram–Schmidt process is used to orthonormalize the different vectors. Further, the following reduced-order stochastic eigenequation is used to solve the stochastic eigenvalue $\lambda_m(\theta)$ and the random vector $\boldsymbol{\phi}_m(\theta)$,

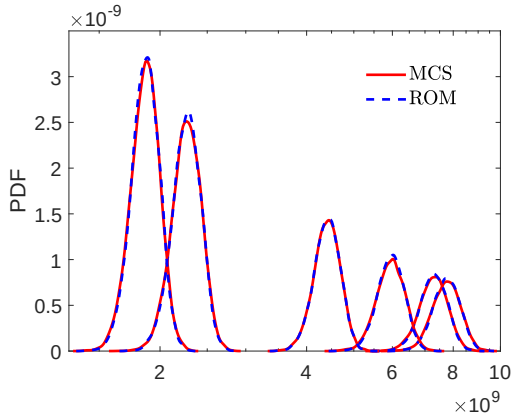
$$\left[\mathbf{D}^{\mathrm{T}}\mathbf{K}(\theta)\,\mathbf{D}\right]\boldsymbol{\phi}_m(\theta) = \lambda_m(\theta)\,\boldsymbol{\phi}_m(\theta). \tag{4}$$

3 Numerical illustration

We consider a three-dimensional mechanical part shown in Fig. 1a and the finite element mesh includes 2062 nodes and 6729 linear tetrahedron elements. Material properties are Poisson's ratio 0.30 and mass density 2000kg/m^3. The Young's modulus $E(\mathbf{x},\theta)$ is modeled as a Gaussian random field with mean function $E_0(x,y) = 1.50\times10^{11}$Pa and exponential covariance function $C(\mathbf{x}_1,\mathbf{x}_2) = \sigma_E^2 \exp(|\mathbf{x}_1 - \mathbf{x}_2|/l_{\mathbf{x}})$, where $\sigma_E = 1.50\times10^{10}$ and $l_{\mathbf{x}}$ are the lengths along x, y, z directions. 20-term truncated Karhunen–Loève expansion is adopted to approximate the random field. 1×10^6 MCS and the proposed method with 20 reduced bases retained are adopted to solve this problem. PDFs of the first six minimum eigenvalues are compared in Fig. 1b, which indicates that the two methods are in good agreement.



(a) Finite element mesh.



(b) PDFs of the first six minimum eigenvalues.

Figure 1: The mechanical part (left) and PDFs of the first six minimum eigenvalues (right).

4 Conclusions

In this paper, a reduced-order method is presented to solve stochastic eigenequations. The original problem is decoupled into deterministic and stochastic spaces. Deterministic eigenequations and reduced-order stochastic equations are solved in the deterministic and stochastic spaces, respectively. The high accuracy of the proposed method is verified using MCS.

5 Acknowledgements

The authors are grateful to the Alexander von Humboldt Foundation and the International Research Training Group 2657 funded by the German Research Foundation (No. 433082294).

References

[1] HJ Pradlwarter, GI Schuëller, GS Szekely. Random eigenvalue problems for large systems. Comput Struct 2002; 80(27-30): 2415-2424.

[2] R Ghanem, D Ghosh. Efficient characterization of the random eigenvalue problem in a polynomial chaos decomposition. Int J Numer Meth Eng 2007; 72(4): 486-504.

[3] ZB Zheng, M Beer, U Nackenhorst. An efficient reduced-order method for stochastic eigenvalue analysis. Int J Numer Meth Eng 2022; 123(23): 5884-5906.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

MORe DWR: Space-time goal oriented error control for incremental POD based ROM

Hendrik Fischer[*,†], **Julian Roth**[*,†], **Amelie Fau**[†] **and Thomas Wick**[*,†]

[*] Institute of Applied Mathematics
Leibniz Universität Hannover
30167 Hannover, Germany
e-mail: {fischer, roth, wick}@ifam.uni-hannover.de

[†]LMPS - Laboratoire de Mecanique Paris-Saclay
Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay
91190 Gif-sur-Yvette, France
e-mail: amelie.fau@ens-paris-saclay.fr

Abstract: In this presentation, we apply the dual-weighted residual method to obtain a certified incremental proper orthogonal decomposition based reduced order model. In order to accomplish this, we introduce a novel approach that marries the space-time reduced order modeling and an incremental proper orthogonal decomposition based basis generation with a goal-oriented error control based on dual-weighted residual estimates. For this purpose, we estimate the error in the cost functional and update the reduced basis if the estimate exceeds a given threshold. This allows an adaptive enrichment of the reduced basis in case of unforeseen changes in the solution behavior which is of high interest in engineering applications. Consequently, we are able to neglect an offline phase and solve the reduced order model directly and –if necessary– update the reduced basis on-the-fly during the simulation with high fidelity finite element solutions. Therefore, we are able to reduce the full-order solves to a minimum, which is demonstrated on numerical tests for the heat and elastodynamics equations.

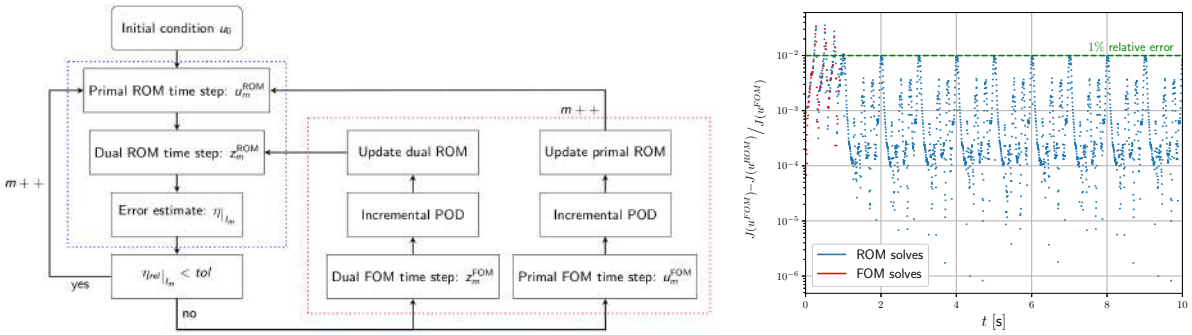
Keywords: reduced order modeling, incremental proper orthogonal decomposition, goal orientated error control, dual-weighted residual method, tensor-product space-time finite elements

1 Introduction

The scope of this talk is to introduce goal oriented error control for reduced order models (ROM) [1] with an adaptive on-the-fly basis generation. Therefore, we utilize a tensor-product space-time discretization [2] and marry the space-time reduced order model and an incremental proper orthogonal decomposition (POD) [3] based basis generation with goal-oriented error control with dual-weighted residual (DWR) estimates [4]. We call the method MORe DWR to highlight the novel combination of model order reduction (MOR) and DWR.

2 MORe DWR

The general structure of the MORe DWR method is illustrated in Figure 1a. For a given initial condition, the ROM is carried out directly. This involves the calculation of an error estimate $\eta|_{I_m}$ on each time interval I_m based on which the decision is made whether the current reduced basis is sufficient or whether it has to be enriched incrementally by a new full order model (FOM) solution. Hence, the finite element solves are reduced to a minimum.



(a) (b)

Figure 1: (a) MORe DWR algorithm and (b) Relative error between FOM and ROM evaluation of the cost functional on each time interval I_m.

We investigate the MORe DWR method on the 2D heat equation with a rotating heat source on the unit square. Figure 1b shows the resulting relative error in evaluating the nonlinear cost functional. At the start, several FOM solves are conducted to fulfill the error threshold. However, it is slightly exceeded in some intervals which reflects the nature of the estimator as distinguished from a bound. Nevertheless, the majority of time intervals are solved by the ROM while fulfilling the error threshold resulting in a speed-up of 7 to 8.

3 Conclusions

We have shown that the presented MORe DWR method achieves notable computational speed-ups while mostly respecting a given error threshold.

4 Acknowledgements

This research is funded by the German Research Foundation (DFG) within the framework of the International Research Training (GRK) 2657 under Grant Number 433082294.

References

[1] Fischer H, Wick T, Fau, A. Reduced-order modeling for parametrized time-dependent Navier-Stokes equations. PAMM, 2022, In press.

[2] Roth J, Thiele JP, Köcher U, Wick T. Tensor-product space-time goal-oriented error control and adaptivity with partition-of-unity dual-weighted residuals for nonstationary flow problems. arXiv:2210.02965, 2022.

[3] Brand M. Fast low-rank modifications of the thin singular value decomposition. Linear algebra and its applications, 415(1):20–30, 2006.

[4] Becker R, Rannacher R. A feed-back approach to error control in finite element methods: basic analysis and examples. East-West J. Numer. Math., 4:237–264, 1996.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Model order reduction techniques for linear and nonlinear dynamical systems

Benjamin Hirzinger[*,†]

[*] International Research Training Group (IRTG) 2657,
Faculty of Civil Engineering and Geodetic Science, Leibniz University Hannover
Hanover, Germany
e-mail: benjamin.hirzinger@irtg2657.uni-hannover.de

[†] Institute of Mechanics and Computational Mechanics,
Faculty of Civil Engineering and Geodetic Science, Leibniz University Hannover
Hanover, Germany

Abstract:

This contribution aims to present and apply model order reduction methods for efficient simulation of nonlinear dynamical systems. Different model order reduction techniques are introduced based on their theoretical basis for linear and nonlinear dynamical systems with the focus on white-box models. Subsequently the proposed methods are utilized on application examples and evaluated in terms of efficiency and accuracy. Finally limits of the reduced order modelling techniques of dynamical systems are discussed.

Keywords: Reduced order modelling, Dynamical systems, Nonstandard features

1 Introduction

Dynamical systems build the basic framework for modelling and control of a vast variety of complex systems in scientific and industrial fields. In civil engineering, responses of e.g. buildings, bridges, and offshore structures under time-dependent excitation are determined by dynamic simulations. Such structural dynamical systems (SDS) commonly described by hyperbolic partial differential equations and solved by using e.g. multi-body dynamic methods or Galerkin finite element method with semi-discretisation often require a large number of simulations for system performance evaluation. Alleviating this computational burden is the primary motivation for deriving reduced models of low dimension that are efficient, fast to solve, and approximate well the underlying high-resolution simulations. A broad set of model order reduction techniques are presented in literature, such as nonlinear manifold methods, Krylov subspace methods, and proper generalized decomposition (PGD), among others, reducing the computational effort [1]. However, for SDSs reduced order modelling is challenging and an active field of research in particular when dealing with nonstandard features such as strong nonlinearities as well as high-dimensional parametric and stochastic spaces.

2 Model order reduction techniques with focus on time-dependent problems

Typically a linear time-dependent systems can be described by system of equations of motion

$$\mathbf{M}\ddot{\mathbf{x}}(t) + \mathbf{C}\dot{\mathbf{x}}(t) + \mathbf{K}\mathbf{x}(t) = \mathbf{F}(t) \tag{1}$$

with mass matrix $\mathbf{M} \in \mathbb{R}^{N,N}$, damping matrix $\mathbf{C} \in \mathbb{R}^{N,N}$, stiffness matrix $\mathbf{K} \in \mathbb{R}^{N,N}$, displacement $\mathbf{x} \in \mathbb{R}^{N}$, and excitation vector $\mathbf{F(t)} \in \mathbb{R}^{N}$ derived by e.g. finite element discretization or

analytical techniques. Transformation of Eq. (1) to state-space results in

$$\dot{\mathbf{y}}(t) = \mathbf{A}\mathbf{y}(t) + \mathbf{B}\mathbf{F}(t) \tag{2}$$

with $\mathbf{y} = \begin{bmatrix}\mathbf{x}\\ \dot{\mathbf{x}}\end{bmatrix}$, $\mathbf{A} = \begin{bmatrix}0 & \mathbf{I}\\ -\mathbf{M}^{-1}\mathbf{C} & -\mathbf{M}^{-1}\mathbf{K}\end{bmatrix}$, and $\mathbf{B} = \begin{bmatrix}0\\ \mathbf{M}^{-1}\end{bmatrix}$. In a linear projection-based framework Eq. (2) is reduced by constructing a transformation to a reduced space [2]. When the projection is created from any basis of a Krylov subspace it can be shown that the moments of the reduced order model and the original model are equal to each other [2]. Considering projection $\mathbf{y}(t) = \mathbf{V}\tilde{\mathbf{y}}(t)$ the reduced order system is given as

$$\mathbf{W}^T\mathbf{V}\dot{\tilde{\mathbf{y}}}(t) = \tilde{\mathbf{A}}\tilde{\mathbf{y}}(t) + \tilde{\mathbf{B}}\mathbf{F}(t), \quad \tilde{\mathbf{A}} = \mathbf{W}^T\mathbf{A}\mathbf{V},\ \tilde{\mathbf{B}} = \mathbf{W}^T\mathbf{B} \tag{3}$$

Nonlinear SDS models can be useful and necessary in particular when it comes to analyse the behaviour of slender structures such as e.g. wind turbine blades and aircraft wings. A representation of a nonlinear dynamical system is achieved by e.g. introducing a history dependent forcing term $\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}})$ on the right-hand side of Eq. (2) reading in state-space $\mathbf{F}(t, \mathbf{y})$ [3]. For SDSs with strong nonlinearities linear projection-based methods (cf. Eq. (3)) have drawbacks. In contrast, spectral subspace manifolds are suitable to construct a reduced order model of SDSs with strong nonlinearities [3].

It is targeted to present the fundamental theory for model order reduction of the briefly introduced systems and to compare the performance with other techniques dealing with model order reduction for SDSs based on application examples for a linear and a nonlinear SDS and to critically discuss the benefits and limitations of model order reduction methods.

3 Conclusions

In this contribution model order reduction methods for linear and nonlinear dynamical systems are introduced and discussed. Reduced order models serve as basis for further performance analysis of engineering structures e.g. structural health monitoring, damage detection, fatigue evaluation, and reliability assessment.

4 Acknowledgements

The author is grateful to the International Research Training Group 2657 (IRTG 2657) funded by the German Research Foundation (DFG) (Grant reference number 433082294).

References

[1] Benner P, Cohen A, Ohlberger M, Willcox K. Model Reduction and Approximation. Society for Industrial and Applied Mathematics; 2017.

[2] Gu C. Model Order Reduction of Nonlinear Dynamical Systems. PhD Thesis, University of California, Berkley; 2011.

[3] Ponsioen S, Pedergnana T, Haller G. Automated computation of autonomous spectral submanifolds for nonlinear modal analysis. Journal of Sound and Vibration 2018; 420:269-295.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A first illustration of a multimodel strategy for coupled multiphysics problems

Floriane Wurtzer, Pierre-Alain Boucard, Pierre Ladevèze and David Néron

Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay, CNRS
LMPS – Laboratoire de Mécanique Paris-Saclay
91190 Gif-sur-Yvette, France
e-mail: {floriane.wurtzer, pierre-alain.boucard, pierre.ladeveze, david.neron}@ens-paris-saclay.fr

Abstract: This contribution proposes a suitable framework for the multimodel simulation of strongly coupled multiphysics problems based on the non-incremental LATIN-PGD method. This strategy relies on introducing an interface between physics, which can be seen as a generalization of the geometrical interfaces between substructures found in domain decomposition. Therefore, the different physics only communicate through this interface (where the coupled equations are satisfied), whereas the monophysical equations are solved separately for each physics. This separate treatment allows using different kinds of models for both physics. A first implementation in the case of strongly coupled 3D thermo-mechanics is presented herein and deals with coupling a full order model (FOM) with a simplified one (reduced order (ROM) or even analytical). The choice of the accommodation space in which these different models communicate is specifically discussed.

Keywords: multiphysics, strong coupling, multimodel, model order reduction, LATIN-PGD

1 Introduction

Since the operation of most modern industrial systems involves interactions between multiple physical phenomena (e.g., mechanical, thermal, electromagnetic), their high-fidelity simulation requires taking their multiphysical behavior into account. In the case of strong coupling, i.e., when all phenomena significantly influence each other, the simulation must address the problem in a coupled way. Commonly used approaches are divided into direct monolithic resolution (treating all physics simultaneously) and partitioning strategies (the physics are treated sequentially but still communicate at each time step) [1]. The presented work focuses on an alternative partitioning method based on the non-incremental LATIN-PGD solver, including the powerful Proper Generalized Decomposition (PGD) ROM technique.

Coupling several physics implies choosing their associated models. Indeed, it may be relevant to couple different types of models [2] (e.g., simplified/fine model, data-based/finite element (FE) model). This contribution proposes a first illustration of a multimodel strongly coupled multiphysics simulation within the framework provided by the LATIN-PGD solver.

2 The LATIN-PGD method

It is a non-incremental iterative approach initially developed for nonlinear evolution problems [3]. In order to deal with multiphysics problems, the method relies on extending the notion of material interface between substructures to an interface between physics on which the physics will interact [4]. The strategy is based on three ingredients:

The first one consists in separating the governing equations into two sets: the linear monophysical but possibly global equations (set $\mathbf{A_d}$) and the local but coupled equations (set $\mathbf{\Gamma}$).

The second idea involves using search directions in a two-stage iterative algorithm to build intermediate solutions belonging to $\mathbf{A_d}$ and $\mathbf{\Gamma}$ alternatively until a sufficient level of convergence has been reached. Thus, each iteration consists of first solving a local in space but coupled system (within the so-called coupled stage) and then solving a global linear system for each physics (during the decoupled stage). Therefore, the simultaneous treatment of both a global and a coupled problem is avoided.

The third one takes advantage of the non-incremental nature of the method, meaning that an approximation of the solution over the whole domain and the entire time interval is provided at each iteration. It is, therefore, highly relevant to apply efficient model reduction techniques based on the PGD to reduce the computational costs of the decoupled stage.

3 First application

The presented method is applied to a strongly coupled 3-dimensional thermo-mechanics problem. First, both physics are solved with standard FE models associated with a PGD decomposition during the decoupled stage. Then, the multimodel aspect is tackled by replacing the FE solution with a simplified model for one of the physics. Special attention is paid to the accommodation of these models on the interface between physics (i.e., where the coupled equations are solved).

4 Conclusions

This work presents a framework adapted for the multimodel simulation of strongly coupled multiphysics problems based on the non-incremental LATIN-PGD solver. The key feature of this approach is the concept of interface between physics. A first illustration is given by coupling a simplified model to a fine one in order to solve a strongly coupled 3D thermo-mechanics problem. First results are very promising in terms of modularity.

References

[1] Felippa CA, Park KC, Farhat C. Partitioned analysis of coupled mechanical systems. Computer Methods in Applied Mechanics and Engineering, 190(24) :3247–3270, 2001.

[2] Néron D, Ben Dhia H, Cottereau R. A decoupled strategy to solve reduced-order multimodel problems in the PGD and Arlequin frameworks. Computational Mechanics, 57(4) :509–521, 2016.

[3] Ladevèze P. Nonlinear Computational Structural Mechanics: New Approaches and Non-Incremental Methods of Calculation. Springer Verlag; 1999.

[4] Néron D, Dureisseix D. A computational strategy for thermo-poroelastic structures with a time-space interface coupling. International Journal for Numerical Methods in Engineering, 75(9) :1053–1084, 2008.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Variational Reduced-Order Thermomechanical Finite Strain Shape Memory Alloy Model for Bistable Microactuators

Shamim Muhammad Babar, Hörsting Marian and Wulfinghoff Stephan*
Institute for Materials Science, Computational Materials Science, Kiel University, 24143 Kiel, Germany
e-mail: mush@tf.uni-kiel.de ; mfs@tf.uni-kiel.de ; swu@tf.uni-kiel.de
* Correspondence: swu@tf.uni-kiel.de

Abstract: In this work, a reduced order thermomechanical finite strain shape memory alloy model is formulated and tested for single shape memory alloy (SMA) based microactuators. The proper orthogonal decomposition (POD) is used to generate the reduced basis that are generated from a precomputed FEM full scale model. These reduced basis can best represent the solution in terms of few displacement and temperature modes. The model order reduction (MOR) obtained in this work is compared with the FEM model and for a single SMA based actuator, the percentage error (E_{per}) were found out to be 0.973% and 0.089% for the displacement and temperature, respectively, with a speedup factor of 9.56.

Keywords: microactuators; shape memory alloy; thermomechanics; reduced-order modeling; proper orthogonal decomposition

1 Introduction

The discussed actuator in this work is based on a concept investigated by Winzek et al. [1]. They explored a combination of SMA and polymer that leads to the actuation of a composite material in a bistable manner. The objective of this paper is to develop a fast and reliable reduced-order actuator model for the FEM model developed in Sielenkämper et al. [2]. The novelty of this work is the application of reduced order modeling (ROM) to the coupled thermomechanical potential, which was first examined by Yang et al. [3]. First, samples of snapshots are generated from full scale FEM solutions for different parameter sets. This so-called offline computation is computationally demanding. Subsequently, a reduced basis that could best represent the full snapshot matrix is obtained through proper orthogonal decomposition. Then, the most significant modes contained in the reduced basis are used to speculate the overall behavior of the nonlinear SMA actuator model.

2 Continuum reduced-order model and results

The temperature and the displacement vector are the unknown state variables for our model. Fourier's heat conduction law is assumed along with dissipative terms. Both state variables are coupled through the following time-discrete potential

$$\pi_\Delta = \psi - (e_n - Ts_n) + \phi_\Delta - \kappa\frac{\Delta t}{2T_n}\|\mathrm{Grad}T\|^2 + \kappa\frac{\Delta tT}{T_n^2}\|\mathrm{Grad}T_n\|^2, \tag{1}$$

where e_n and s_n are the internal energy density and entropy density at time t_n, respectively, κ is the heat conductivity, ψ is the free energy density, ϕ_Δ is the dissipation potential in time-discrete format, T is the temperature, and the last two terms in Eq. 1 are related to heat conduction in the body. The weak form for the linear momentum balance in reduced-order format is given as

$$\delta_\xi \Pi_\Delta = \sum_{i=1}^{N_u} \delta\xi_i \underbrace{\left[\int_{\mathcal{B}_0} \boldsymbol{\tau} : \mathbf{g}_i^s \mathrm{d}V - \int_{\partial\mathcal{B}_{0t}} \hat{\boldsymbol{t}} \cdot \boldsymbol{\psi}_i \mathrm{d}S - \int_{\mathcal{B}_0} \rho_0 \boldsymbol{b} \cdot \boldsymbol{\psi}_i \mathrm{d}V\right]}_{R_i^u}, \tag{2}$$

where $\boldsymbol{\tau} = \boldsymbol{F}\boldsymbol{S}\boldsymbol{F}^T$ is the Kirchhoff stress tensor, $\boldsymbol{S} = \boldsymbol{F}^{-1}\boldsymbol{P}$ is the second Piola–Kirchhoff stress tensor, $\mathbf{g}_i^s$ is the symmetric part of $\boldsymbol{G}_i\boldsymbol{F}^{-1}$, with $\boldsymbol{G}_i = \mathrm{Grad}\boldsymbol{\psi}_i(\boldsymbol{X})$, $\hat{\boldsymbol{t}}$ is the traction vector, $\boldsymbol{b}$ is the body force, ρ_0 is the reference mass density, ξ_i is the mode coefficient, ψ_i are the displacement modes. Likewise, the weak form of the energy balance can be expressed as

$$\delta_T \Pi_\Delta = \sum_{m=1}^{N_T} \delta\mu_m \underbrace{\left[\int_{\mathcal{B}_0} \left(\left(\frac{\partial \pi_\Delta}{\partial T} + \frac{\Delta t}{T_n} w\right)\chi_m + \frac{\partial \pi_\Delta}{\partial \mathrm{Grad}T} \cdot \boldsymbol{W}_m\right)\mathrm{d}V - \int_{\partial\mathcal{B}_{0\mathrm{Q}}} \frac{\partial \pi_\Delta^s}{\partial T}\chi_m \mathrm{d}S\right]}_{R_m^T}, \tag{3}$$

where $\boldsymbol{R}_i^u$ and $\boldsymbol{R}_m^T$ are the residuals for the mechanical and thermal subproblems, respectively, χ_m are the temperature modes and $\boldsymbol{W}_m = \text{Grad}\chi_m(\boldsymbol{X})$. Now, solving Equations 2 and 3 resulted in the graphs for the displacement and temperature as shown in Figure 2 for the points circled as green in Figure 1(right).

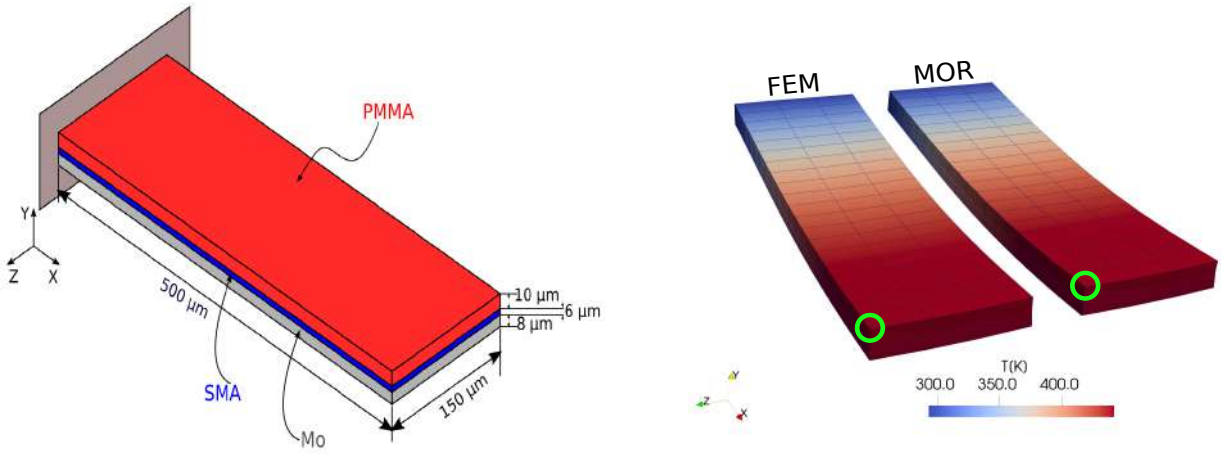


Figure 1: Dimensions of the actuator assembly, which is clamped at the left side. The red layer is polymer, blue is SMA and gray is molybdenum. (**left**). FEM and MOR result comparison for temperature for an "untrained" parameter set with 10 modes ($E = 331$ MPa and $\nu = 0.35$ (**right**).

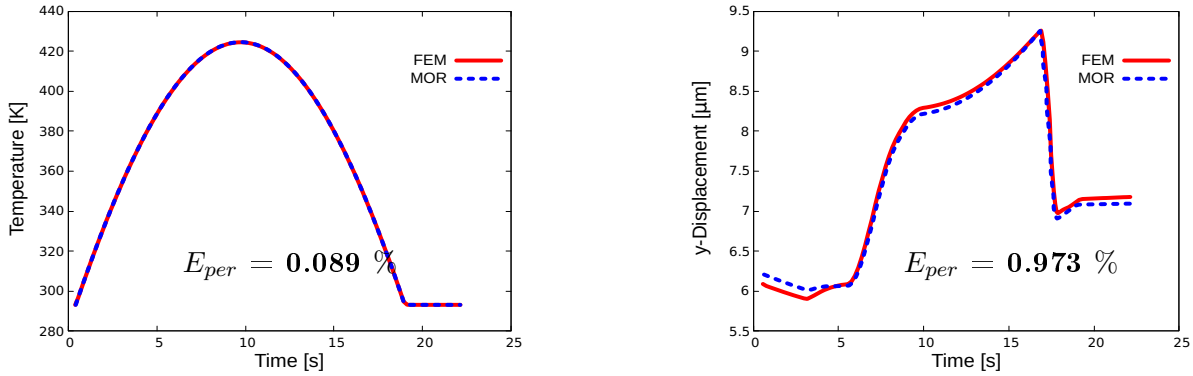


Figure 2: FEM and MOR comparison for displacement and temperature for one heat cycle (**left**). Temperature graph with 10 modes. Displacement graph with 34 modes (**right**).

3 Conclusions

As a major novelty, the reduced-order model in this work is derived from an incremental thermomechanical potential, which ensures a symmetric tangent, and thus allows for efficient solvers and may enable a mathematical model analysis and the employment of enhanced solution methods. The ROM is tested for a single actuator example. It was shown from the numerical examples that the model can predict the properties of a parameterized actuator model with less computational effort and controlled accuracy.

References

[1] Winzek, B.; Schmitz, S.; Rumpf, H.; Sterzl, T.; Hassdorf, R.; Thienhaus, S.; Feydt, J.; Moske, M.; Quandt, E. Recent developments in shape memory thin film technology. *Mater. Sci. Eng. A* **2004**, *378*, 40–46.

[2] Sielenkämper, M.; Wulfinghoff, S. A thermomechanical finite strain shape memory alloy model and its application to bistable actuators. *Acta Mech.* **2022**, *233*, 3059–3094.

[3] Yang, Q.; Stainier, L.; Ortiz, M. A variational formulation of the coupled thermo-mechanical boundary-value problem for general dissipative solids. *J. Mech. Phys. Solids* **2006**, *54*, 401–424.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

An efficient sampling method for reduced order modelling of composite laminates

Imran Omar*, Iannucci Lorenzo

* Department of Aeronautics
Imperial College London
London, United Kingdom
e-mail: oai15@ic.ac.uk

Abstract: Ply layup optimisation studies used for composite aircraft structures can be accelerated through the use of reduced order modelling of finite element simulations. For such application, it is important to understand the effect of varying the laminate stacking sequence on material behaviour, such as damage initiation. There are multiple feature spaces that can be used to represent laminate layup distributions, and therefore if we are to sample across multiple feature spaces, the design of experiment must effectively deal with this highly dimensional problem. Furthermore, generation of a laminate stacking sequence given a sampled laminate distribution often requires costly genetic algorithms in a seperate post-processing step. In this investigation, we devise an algorithmic sampling method to deal with this highly dimensional problem and simultaneously generate laminate stacking sequences without involving costly genetic algorithm processes. This method uses a variant of Latin Hypercube Sampling to sample within one feature space and the maximin criterion to maximise the Euclidean distance between samples in another feature space. Composite design guidelines such as the 10% rule are embedded in this method to generate feasible plies for laminates of varying thickness. Results show samples that are well distributed in both feature spaces.

Keywords: Design of Experiment, Composites, Laminate Stacking Sequence, Maximum Projection, Maximin

1. Introduction

Two feature spaces are commonly used in the preliminary design of composite laminates to represent the layup distribution [1,2]. The first space, which we refer to as the descriptor space, varies the number of plies and the percentage of plies in each of the classic quad angle. A common design rule within this space is the 10 % rule that requires there to be no less than 10 % of plies (and no more than 90 % of plies) in any of these classic quad angles [3]. The second space, we refer to as the laminate parameter space, is derived from the effect of stacking sequence on the 'ABD' matrix. There are 12 laminate parameters, however, for symmetric, balanced, classic quad laminates this reduces to 4 laminate parameters (L1-L4) [1]. Ply layup optimisation studies [1,2] have commonly sampled from either one of these spaces but not across both, and therefore there is not guarantee that samples are well distributed in both spaces. Also, to define a laminate stacking sequence for each sample, a subsequent step using a genetic algorithm is often required. However, in this investigation we generate a design of experiment method that samples across both the descriptor and laminate parameter space simultaneously, without the need of genetic algorithms to generate a corresponding laminate stacking sequence.

2. Method

The design of experiment method developed uses a variant of Latin hypercube sampling called Maximum Projection [4]. Latin hypercube sampling is a stratified sampling technique that doesn't suffer the curse of dimensionality. The maximum projection variant maximises

the projection of each sample within the dimensions of the sampling space, ensuring a better distributed design of experiment. This maximum projection sampling technique is applied to the descriptor space with inversion sampling to ensure that the percentages of plies add up to 100 % and with samples which violate the 10 % rule also being filtered out. For each sample, we derive 1000 feasible laminate stacking sequences. We then use the maximin criterion to select the laminate stacking sequence that maximises the Euclidean distances between samples in the lamination parameter space.

3. Results and Conclusion

Figure 1 shows the distribution of 100 samples generated using this method across the feasible regions of both feature spaces. The laminate stacking sequences have been successfully sampled without slow genetic algorithms and are well distributed in the descriptor space (due to the maximum projection sampling scheme) and well distributed in the laminate parameter space (due to the maximin criterion). These samples may be used to generate training data for reduced order modelling techniques such as machine learning, in order to accelerate ply layup optimisation.

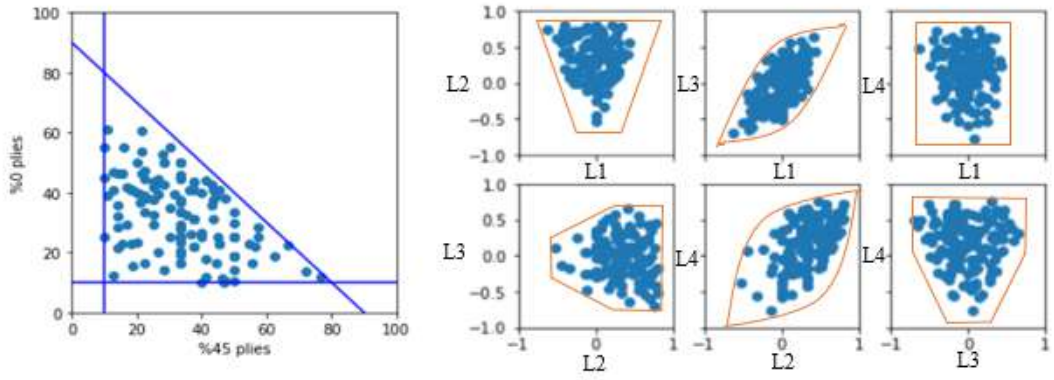


Figure 1. Samples bounded in feasible regions in both the descriptor space (left) and laminate parameter space (right).

References

[1] Albazzan, M. et al. “Efficient design optimization of nonconventional laminated composites using lamination parameters: A state of the art”. Composite Structures 2019.

[2] Liu, X. et al. “Two-level layup optimization of composite laminate using lamination parameters”. Composite Structure 2019.

[3] Niu, MC-Y. Composite Airframe Structures: Practical Design Information and Data. Hong Kong: Conmilit; 1992.

[4] Joseph, V. R., et al. “Maximum Projection Designs for Computer Experiments”. Biometrika, 102, 371-380 (2015).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A multisurface damage plasticity model for masonry

Bertani Gregorio[*], Patruno Luca[*], D'Altri Antonio Maria[*†], Castellazzi Giovanni[*] and de Miranda Stefano[*]

[*] Dipartimento di Ingegneria Civile, Chimica, Ambientale e dei Materiali (DICAM), Università di Bologna, Italy
e-mail: gregorio.bertani2@unibo.it, luca.patruno@unibo.it, am.daltri@unibo.it, giovanni.castellazzi@unibo.it, stefano.demiranda@unibo.it

[†] Department of Civil and Environmental Engineering, Princeton University, USA
e-mail: ad4706@princeton.edu

Abstract: Due to the complex and nonlinear mechanical behaviour, the analysis of masonry structures usually relies on numerical simulations. For such aim, block-based models and continuum models are the most widely adopted approaches. In block-based models, masonry texture is explicitly represented, leading to accurate models able to represent all the prominent failure mechanisms of masonry, such as joint failure and masonry crushing. However, their computational burden is high and prohibitive for applications to large-scale structures. Consistently, continuum models are still widely employed, although their accuracy substantially depends on the choice of the most appropriate constitutive model. In this contribution, we propose a continuum model for masonry derived through homogenization of a nonlinear block-based model with damaging blocks and frictional-cohesive joints. By relying on a multisurface strength domain, the proposed model is able to explicitly account for all the masonry failure mechanisms, also paving the way to damage classification. Particularly, focus is here made on the damage evolution law inherited from the block-based model. The model is implemented in a finite element code and tested on some simple structural examples, limiting to regular periodic masonry. Numerical results are also compared with those obtained with a detailed finite element block-based model.

Keywords: Masonry, Continuum model, Block-based model, Constitutive model, Numerical simulations

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Multi-Unit discretization approach for nonlinear analysis of URM walls

Di Lallo Ylenia[*], Rapone Davide[*], Masciotta Maria Giovanna[*] and Brando Giuseppe[*]

[*] Department of Engineering and Geology (INGEO)
University "G. d'Annunzio" of Chieti-Pescara
Pescara, Italia
e-mail:ylenia.dilallo@unich.it

Abstract: This paper discusses the validation process of a new Multi-Unit Discretization (MUDis) approach developed for simulating the in-plane behaviour of masonry structures under horizontal actions. The peculiarity of the procedure lies in the possibility to discretize periodic masonry walls using a limited number of repeated modules covering more than a single unit of masonry, thus greatly reducing the sources of nonlinearity and minimizing the computational effort. The modules are made of polygonal units separated by interface elements whose pre-established layout allows to reproduce the typical in-plane collapse mechanisms of masonry walls subjected to lateral loads. The mechanical parameters of the new interface elements are described through the "combined cracking-shearing-crushing" model, widely used in the FEM-based simplified micromodeling of masonry structures. In order to adapt this constitutive model to the MUDis-based modelling, three of these parameters have been suitably modified by the Authors through parametric formulas.

Keywords: Masonry modelling; Nonlinear analysis; Masonry buildings; pushover analysis; FEM analysis

1. Introduction

Masonry buildings represent a significant part of the worldwide historical architectural heritage. Given the complexity of these structures and their notable vulnerability against earthquake actions, it is very important to find efficient methods for assessing their highly indeterminate behaviour and possible damage mechanisms due to seismic events [1]. In this context, the definition of suitable modelling strategies capable of providing accurate results with a sustainable computational burden remains a pivotal issue [2] and several authors are trying to develop increasingly simplified models to achieve this purpose [3]. Following this line of research, the present work outlines a new multi-unit discretization approach (MUDis) aimed at making the seismic analysis of masonry structures far more expedite than simplified micro-modelling procedures, without compromising the accuracy of the results. The validation of the MUDis approach, already performed on two-dimensional masonry panels, is currently being extended to more complex masonry structures in order to test its applicability and reliability in case of real full-scale buildings.

2. The proposed MUDis procedure

In the MUDis-based modelling procedure, periodic masonry walls are numerically represented by a discretized pattern of multi-unit (MU) quadrangular modules. These modules are made of four elastic polygonal units separated by nonlinear zero-thickness interface surfaces (Figure 1a), representative of the nonlinear behaviour of both mortar joints and mortar-brick interface surfaces, where all basic types of masonry failure phenomena can occur. This layout was determined in order to closely approximate the most common in-plane failure mechanisms observed in masonry panels subjected to vertical and horizontal actions [4]. The well-known CI (composite interface) constitutive model proposed by Lourenço and Rots [5], which considers a Coulomb friction model for shear failure, combined with a tension cut-off for the failure in tension and an elliptical cap for the

compressive failure, is chosen for the mechanical description of the new interfaces. This model, also known as "combined crack-shearing-crushing model", was purposely designed for simplified micro-modelling strategies. Hence, to adapt its formulation to the MUDis-based modelling, transformation relationships based on evolutionary polynomial regression are derived to estimate the most influential mechanical parameters of the proposed model interfaces (tensile strength, cohesion, and friction angle). Interested readers can refer to [4] for details.

3. Validation and conclusions

To prove the reliability and replicability of the modelling strategy, an in-depth validation process is being carried out on progressively complex structures. After testing the procedure on masonry panels, the validation has now been extended to two-dimensional full-scale walls, such as the URM façade of the two-story building tested on the shaking table at the University of Pavia [6]. The numerical analyses are carried out with the MIDAS-FEA software [7], which allows considering the CI model for the interface elements. The case study has been faithfully reproduced both in terms of construction details and loading protocols: the wall is discretized with a set of 250 mm side modules represented through six-node triangular shell elements with three Gaussian integration points, separated by two-node zero-thickness interfaces elements. The results from the nonlinear static analysis performed to simulate the experimental quasi-static tests corroborate the suitability of the MUDis approach in reproducing the in-plane behaviour of masonry walls under horizontal actions (Figure 1). The next step of the validation will be devoted to verifying the applicability of the proposed model to the simulation of the out-of-plane behaviour of masonry walls.

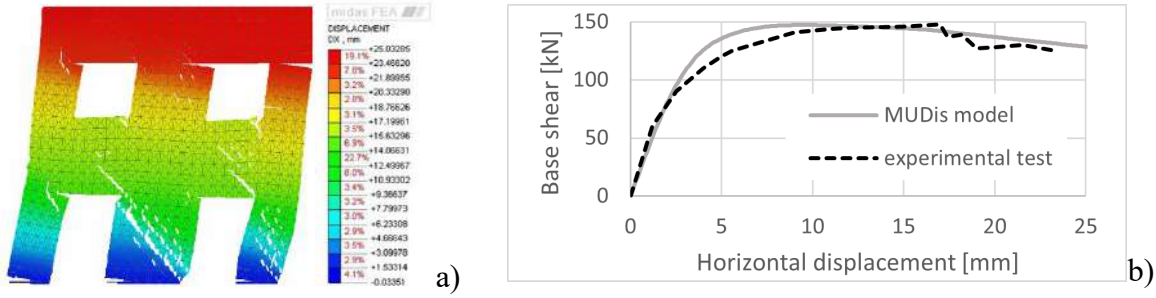


Figure 1. a)ultimate displacement of numerical model; b)experimental vs numerical load-displacement curves

References

[1] Facconi L, Minelli F, Vecchio FJ. Predicting uniaxial cyclic compressive behavior of brick masonry: new analytical model. Journal of Structural Engineering, 2018; 144(2):04017213.
[2] D'Altri AM, Sarhosis V, Milani G. Modeling Strategies for the Computational Analysis of Unreinforced Masonry Structures: Review and Classification. Archives of Computational Methods in Engineering, 2020; 27:1153-1185.
[3] Malomo D, Dejong MJ. A Macro-Distinct Element Model (M-DEM) for simulating the in-plane cyclic behavior of URM structures. Engineering Structures, 2021; 227:111428.
[4] Brando G, Rapone D, Spacone E, Masciotta MG. MUDis: A low computational effort Multi-Unit Discretization procedure for modelling masonry walls with periodic arrangement. Structures, 2022; Vol. 43, pp 1380-1406, ISSN 2352-0124.
[5] Lourenço PB, Rots JG. Multisurface Interface Model for Analysis of Masonry Structures. Journal of Engineering Mechanics, 1997; Vol. 123, no. 7, pp. 660–668.
[6] Magenes G, Kingsley G R, Calvi GM. Seismic testing of a full-scale, two-story masonry building: test procedure and measured experimental response. Consiglio Nazionale delle Ricerche (CNR) - Gruppo Nazionale per la Difesa dai Terremoti - Technical Report 3.0. Pavia, Italy. [in Italian], 1995.
[7] M.F. CSPFEA, "Nonlinear & detail finite element analysis system for civil structures", User Manual, FEA 2016.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Shell-3D multiscale model for masonry based on Uniform and Non-Uniform TFA procedures

Gatta Cristina*, Addessi Daniela*, Di Re Paolo* and Sacco Elio†

* Department of Structural and Geotechnical Engineering
Sapienza University of Rome
Rome, Italy
e-mail: cristina.gatta@uniroma1.it,daniela.addessi@uniroma1.it,paolo.dire@uniroma1.it

† Department of Structures for Engineering and Architecture
University of Naples Federico II
Naples, Italy
e-mail: elio.sacco@unina.it

Abstract: This work focuses on reduced-order multiscale models for the analysis of masonry elements with periodic texture. The Transformation Field Analysis (TFA) procedure is adopted to determine the constitutive response of the homogeneous shell analyzed at the macroscale, on the basis of the response of the representative masonry unit cell (UC), studied at the microlevel by adopting the three-dimensional Cauchy continuum. The UC consists of elastic bricks bounded by interfaces representing mortar joints, where damaging and frictional mechanisms occur. In the spirit of the TFA homogenization, the nonlinear interfaces are discretized into regions where prescribed variation of the inelastic quantities is assumed. Advantages and disadvantages of considering uniform and non-uniform distributions of the inelastic variables over each region are studied by performing numerical applications at both material and structural levels. The results obtained with the proposed model are compared with micromechanical and experimental reference solutions.

Keywords: Masonry, TFA homogenization, multiscale, damage-friction, interfaces

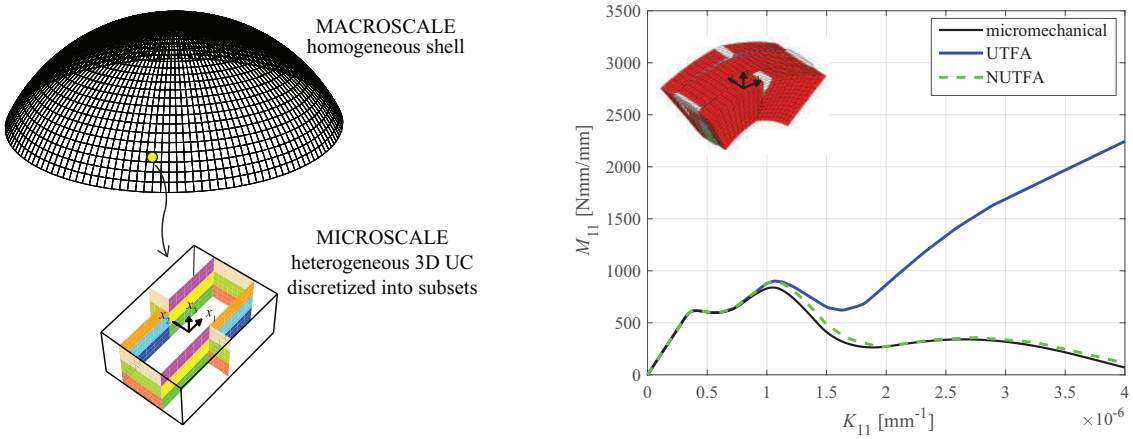
1 Introduction

The most fascinating Italian and European landscapes are composed by masonry structures that suffered damage due to aging and/or extreme loading. Hence, assessment of their safety conditions is a challenging task for the scientific community. Many numerical models, ranging from simplified to sophisticated, have been proposed to analyze masonry [1]. Among them, multiscale formulations are recognized as an effective and powerful tool, as they allow accurate mechanical/geometrical descriptions. In this framework, reduced-order models have been developed, commonly relying on the Transformation Field Analysis (TFA) procedure to determinate the homogenized response of the heterogeneous masonry material.

2 TFA-based multiscale modeling approach

Response of flat and curved masonry elements characterized by regular arrangement of bricks and mortar joints is analyzed by adopting the multiscale formulation proposed in [2]. This links a homogeneous Mindlin-Reissner shell model at the macroscale to a three-dimensional (3D) description of the masonry representative unit cell (UC) at the microscale (Fig. 1(a)).

The TFA procedure is adopted to address the nonlinear homogenization problem. Hence, the UC interfaces representing mortar joints are divided into subdomains, called subsets, where the nonlinear phenomena can occur with pre-assumed variations. Particularly, two TFA versions are developed and compared, considering Uniform (UTFA) and Non-Uniform (NUTFA) distributions of the inelastic quantities over each subdomain. The model is implemented in a finite element code and used to perform several numerical applications.



(a) (b)

Figure 1: (a) shell-3D multiscale model; (b) response of a running bond UC under bending curvature.

3 Conclusions

The analyses show that the model satisfactorily reproduce micromechanical and experimental responses of masonry UCs and structural members. It is proved that the NUTFA improves predictions of the UTFA model, if the same subset partition is considered (Fig. 1(b)). However, the NUTFA increases the computational complexity, as it requires to solve the damage and friction problems in further points identified in each subset according to the non-uniform profile assumed for the inelastic variables.

4 Acknowledgements

D.A. and C.G. acknowledge the grant PNRR PE5-Spoke 7 (CUP: B53C22003780006).

References

[1] D'Altri AM, et al. Modeling strategies for the computational analysis of unreinforced masonry structures: review and classification. Arch Comput Methods Eng 2020;27:1153-1185.

[2] Addessi D, Di Re P, Gatta C, Sacco E. Multiscale analysis of out-of-plane masonry elements using different structural models at macro and microscale. Comput Struct 2021;247:106477.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Phase field approach for the analysis of masonry structures: a comparison with pre-existing simulations

Rodella Andrea, Di Re Paolo and Gatta Cristina

Department of Structural and Geotechnical Engineering (DISG)
Sapienza University of Rome
Rome, Italy
e-mail: andrea.rodella@uniroma1.it, paolo.dire@uniroma1.it, cristina.gatta@uniroma1.it

Abstract: This work presents a phase field computational model for unreinforced masonry structures. The model accounts for brittle fracture in the mortar joints while the bricks obey, for simplicity, a linear elastic constitutive law. The theoretical formulation is presented in a variational framework: the functional, to be minimized, represents the total energy of the composite. The numerical solution scheme is based on a staggered algorithm, which alternatively solves the elastic and the damage problems. We then apply the methodology to numerical examples and compare the results to those in the literature.

Keywords: Phase field, Fracture, Masonry, Variational formulation

1 Introduction

In the last two decades, the phase field approach gained popularity in the scientific community for its ability to accurately describe different mechanical phenomena, as, for instance, the brittle fracture [1] and the material remodeling [2].

In the realm of masonry, the method can be used to simulate the behavior of structures under various quasi-static loading conditions and then study the effects of damage onset and propagation up to structural failure. Furthermore, the phase field method allows for the modeling of complex domains; it can be implemented to predict the behavior of masonry structures at different scales, even in the case of important discontinuities of the fields, i.e., displacement's jumps between the edges of a crack.

Starting from the research findings presented in [3], this work aims to understand the predictive capabilities of the phase field model applied to a representative masonry unit cell under different load conditions.

2 Energetic formulation and numerical implementation

A phase field model typically describes the evolution of a given system's internal state by introducing a scalar quantity, named the *phase field*, that varies continuously over the material domain. The energetic formulation of the problem takes advantage of the generalized standard materials theory [4], on which the phase field is based. It introduces a set of internal variables on which the elastic energy density and dissipation potential depend. In this specific case, the variables which describe the state are: (i) the displacement $\mathbf{u}$, a vector field that can suffer discontinuities, and (ii) the damage α, a continuous scalar field varying from

0, sound material, to 1, completely damaged material. The solution consists of finding the minimum of the total energy $\mathcal{E}$ with respect to the state variables as follows:

$$\{\mathbf{u}, \alpha\} = \min_{\mathbf{u},\alpha} \mathcal{E} = \min_{\mathbf{u},\alpha} \left[\int_{\Omega_b} \frac{1}{2} \mathbb{C}_b \nabla \mathbf{u} \cdot \nabla \mathbf{u} + \int_{\Omega_m} \frac{1}{2} (1-\alpha)^2 \mathbb{C}_m \nabla \mathbf{u} \cdot \nabla \mathbf{u} + w_m \left(\alpha + \frac{(\eta \nabla \alpha)^2}{2} \right) \right] \tag{1}$$

where $\mathbb{C}_b$ and $\mathbb{C}_m$ are respectively the brick and mortar stiffness tensors, w_m is a constant related to the toughness of the mortar and η represent the characteristic crack length.

The variational formulation is particularly suitable for implementation in FEniCSx. Furthermore, the solver consists of an alternative minimization with respect to the internal variables until convergence.

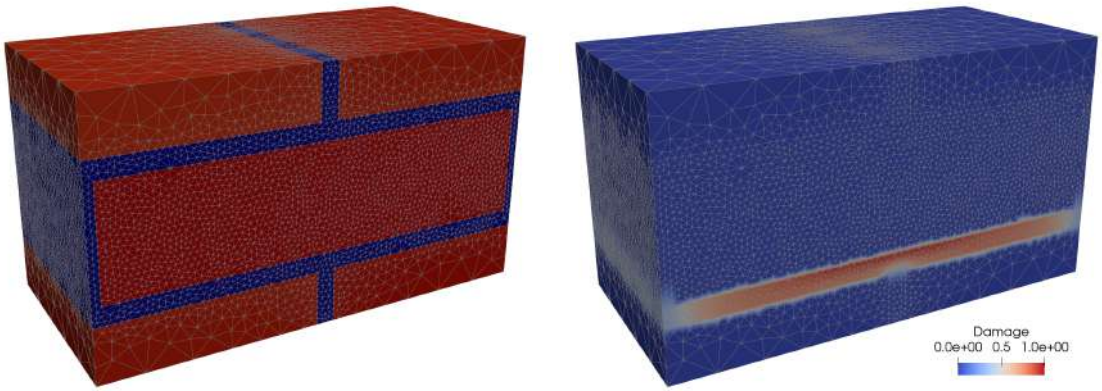


Figure 1: Mesh of the masonry representative unit cell. (left) The domain concerning the bricks, Ω_b, is represented in red color while blue highlight the mortar domain, Ω_m. (right) The damage field corresponding to confined vertical traction. Damaged material is represented in red while sound material in blue.

3 Conclusion and future perspectives

The work investigates the performance of the phase field modeling approach when applied to the analysis of masonry structures. Despite the simplicity of the proposed model, accounting only for the brittle fracture in mortar joints, the comparison with the literature results obtained with existing methods appears promising.

References

[1] Francfort GA, Marigo JJ. Revisiting brittle fracture as an energy minimization problem. J Mech Phys Solids 1998;46:1319-1342.

[2] Favata A, Rodella A, Vidoli S. An internal variable model for plastic remodeling in fibrous materials. Eur J Mech A Solids 2022;96:104718.

[3] Addessi D, Di Re P, Gatta C, Sacco E. Multiscale analysis of out-of-plane masonry elements using different structural models at macro and microscale. Comput Struct 2021;247:106477.

[4] Mielke A. A Mathematical Framework for Generalized Standard Materials in the Rate-Independent Case. In: Helmig, R., Mielke, A., Wohlmuth, B.I. (eds) Multifield Problems in Solid and Fluid Mechanics. Lecture Notes in Applied and Computational Mechanics, vol 28. Springer

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

On the use of Finite and Discrete Macro-Element modelling approaches for the nonlinear static analysis of URM walls

Federica Vadalà[1], Luis C. M. da Silva[2], Ivo Caliò[3], Paulo B. Lourenço[1]

[1] Department of Civil Engineering (DEC)
Universidade do Minho
Guimarães, Portugal
e-mail: federicavadala03@gmail.com, pbl@civil.uminho.pt

[2] Department of Architecture, Built Environment and Construction Engineering (ABC)
Politecnico di Milano
Milan, Italy
e-mail: luiscarlos.martinsdasilva@polimi.it

[3] Department of Civil Engineering and Architecture (DICAR)
University of Catania
Catania, Italy
e-mail: icalio@dica.unict.it

Abstract:

Keywords: Unreinforced masonry, Parameters calibration, In-plane behaviour, Discrete macro-element method, Micro-FE models

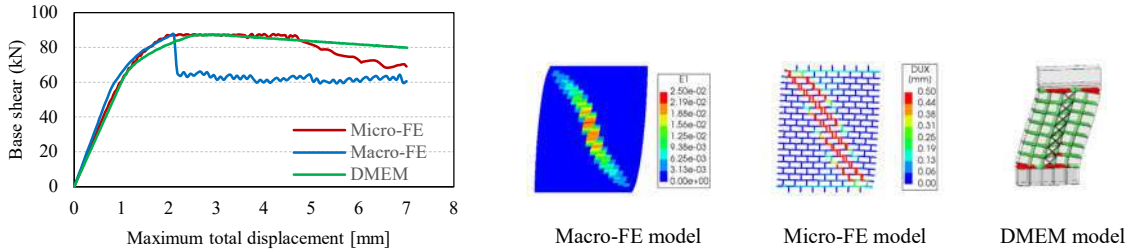
1. INTRODUCTION

Several modelling strategies have been presented in the literature for the structural assessment of masonry structures. The accuracy and computational time vary according to the material-scale under representation and the modelling strategy adopted, i.e., through an equivalent continuum, macro-block or discrete-based models. Various research works prove how the discrepancy of results can be significant [1], [2], unless consistent assumptions among the modelling strategies are made when defining the corresponding input parameters. Studies over a systematic comparison between modelling strategies are still few in the literature [3], [4]. Thence, this paper is focused on the investigation of both a Discrete Macro-Element and Finite Element model when applied within nonlinear static analyses on masonry walls. The goal is to provide a rational use of the models, in such a way that the input mechanical properties characterizing the micro-FE models, which implicitly incorporate the orthotropic nature of the masonry media, are calibrated to serve as input to the DMEM model.

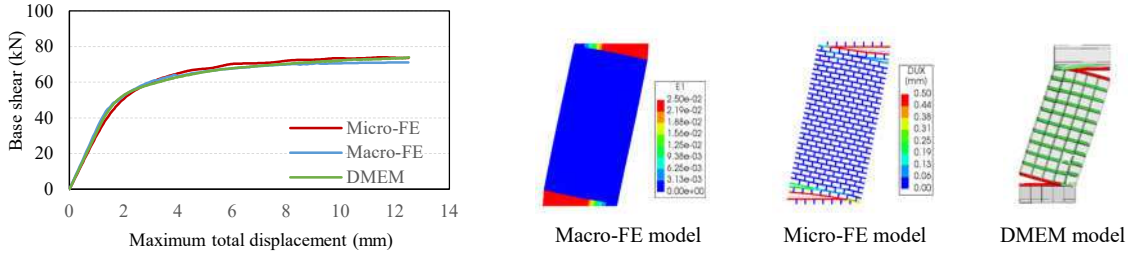
2. RESULTS AND CONCLUSIONS

A cross-calibration has been initially performed at the scale of single panels and with different aspect ratios. This allowed to have control over the parameters that govern the response, while ensuring a good correspondence between the FEs and Discrete models in terms of maximum strength, displacement capacity and failure mechanism. The calibration of the panel stiffness has been performed, as well as the panel strength for different levels of vertical pre-compression ($\sigma_v/f_c = 0 \div 0.8$). In all cases, the analytical strength criteria served as reference [5]. The parameters found through calibration ensured a good fitting in

terms of capacity curves and damage patterns, as shown in Figure 1. Furthermore, the reproduction of the diagonal shear behaviour is achieved. Therefore, a good agreement between the different approaches has been obtained for a 2D regular wall, in which the material parameters determined for the masonry panels have been adopted.



(a) squat wall (height/base=1.35)



(b) slender wall (height/base=2.0)

Figure 1. Obtained pushover curves and crack patterns ($\sigma_v/f_c = 0.1$).

References

[1] A. Aşıkoğlu, G. Vasconcelos, P. B. Lourenço, and B. Pantò, "Pushover analysis of unreinforced irregular masonry buildings: Lessons from different modeling approaches," *Eng. Struct.*, vol. 218, p. 110830, Sep. 2020, doi: 10.1016/J.ENGSTRUCT.2020.110830.

[2] F. Parisse, R. Marques, S. Cattari, and P. B. Lourenço, "Finite Element and Equivalent Frame modeling approaches for URM buildings: Implications of different assumptions in the seismic assessment," *J. Build. Eng.*, vol. 61, p. 105230, Dec. 2022, doi: 10.1016/J.JOBE.2022.105230.

[3] A. M. D'Altri, F. Cannizzaro, M. Petracca, and D. A. Talledo, "Nonlinear modelling of the seismic response of masonry structures: Calibration strategies," *Bull. Earthq. Eng.*, vol. 20, no. 4, pp. 1999–2043, Mar. 2022, doi: 10.1007/S10518-021-01104-1.

[4] S. Cattari and G. Magenes, "Benchmarking the software packages to model and assess the seismic response of unreinforced masonry existing buildings through nonlinear static analyses," *Bull. Earthq. Eng.*, vol. 20, no. 4, pp. 1901–1936, Mar. 2022, doi: 10.1007/S10518-021-01078-0/FIGURES/20.

[5] V. Turnšek and P. Sheppard, " The shear and flexural resistance of masonry walls. Some experimental results on the strength of brick masonry walls," in *International research conference on earthquake engineering*, 1980, pp. 149–156.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical simulation of masonry wall structures using macro and mesoscale models

Luca Bomben[a], Lorenzo Macorini[b], Corrado Chisari[c], Claudio Amadio[a], Bassam Izzudin[b]

[a] Department of Engineering and Architecture – University of Trieste, Trieste, Italy
e-mail: luca.bomben@phd.units.it

[b] Department of Civil and Environmental Engineering, Imperial College London, South Kensington Campus, London, UK

[c] Department of Architecture and Industrial Design, Università della Campania "Luigi Vanvitelli", Aversa, Caserta, Italy

Abstract: This work investigates the nonlinear response up to collapse of unreinforced masonry (URM) wall components and structures under seismic loading. Finite element descriptions formulated according to different scales of representation for masonry, which comprise detailed mesoscale and more efficient macroscale and macroelement models, are used. The purpose of the research is to evaluate the different models based on the prediction of the hysteretic response under cyclic loading conditions representing earthquake actions. To this aim experimental tests from the literature, including two masonry panels with different aspect ratios and a large two-storey height perforated wall, are analysed. The results from the numerical simulations performed using the macro and mesoscale models are compared assessing not only their ability to represent strength and stiffness degradation and the amount of dissipated energy, but also the ease of definition and calibration of the model material parameters.

Keywords: Nonlinear seismic analysis; cyclic response; unreinforced masonry; finite element modelling.

Extended abstract

Over recent years, a considerable effort has been devoted to the development of numerical models for the simulation of the seismic response of unreinforced masonry (URM) structures. Accurate models are critical for realistic assessment under earthquake loading, where the response is particularly complex due to masonry anisotropic nature and highly nonlinear behaviour.

In current practice, seismic assessment of existing masonry building structures is generally conducted by performing nonlinear static analysis under increased lateral loading (pushover analysis). While such an analysis procedure provides a satisfactory estimate of load capacity and global ductility, it does not explicitly allow for the distinctive hysteretic behaviour under cyclic loading conditions, which ultimately determine the actual seismic response up to collapse.

This work investigates the behaviour of masonry wall components and structures considering the response characteristics under cyclic loading conditions. Finite element models based on different scales of representation for masonry are compared simulating the response of masonry wall components and systems. The adopted models include detailed mesoscale models [1], which account for the masonry bond explicitly, representing masonry units and mortar joints independently with elastic solid elements and nonlinear interfaces. More efficient masonry macroscale and macroelement models are also considered. In the former case a continuum representation for masonry, which is assumed as a uniform and isotropic material, is adopted allowing for material nonlinearity using a damage-plasticity constitutive model [2]. In the latter case, on the other hand, a large portion of masonry wall

components is represented with sophisticated macroelements consisting of deformable blocks interacting through cohesive interfaces improving computational efficiency.

The numerical predictions are validated through comparisons against previous experimental tests. More specifically, two masonry panels characterised by different aspect ratios and failure modes and an entire two-storey façade wall have been investigated by performing nonlinear analysis under cyclic loading conditions.

In this study, particular emphasis is given to the definition of the material properties required by the various modelling approaches based on the results from standard material tests. A parametric study is also conducted by varying the most critical parameters for each modelling approach within a realistic range of values. Mechanical parameters determining the monotonic behaviour are initially calibrated to reproduce the envelope of the experimental cyclic response. Subsequently, the parameters governing the hysteretic behaviour are estimated with the aim of predicting the actual load-displacement experimental cycles in terms of the evolution of the dissipated energy and the activation of the failure mechanisms observed in the tests (Figure 1).

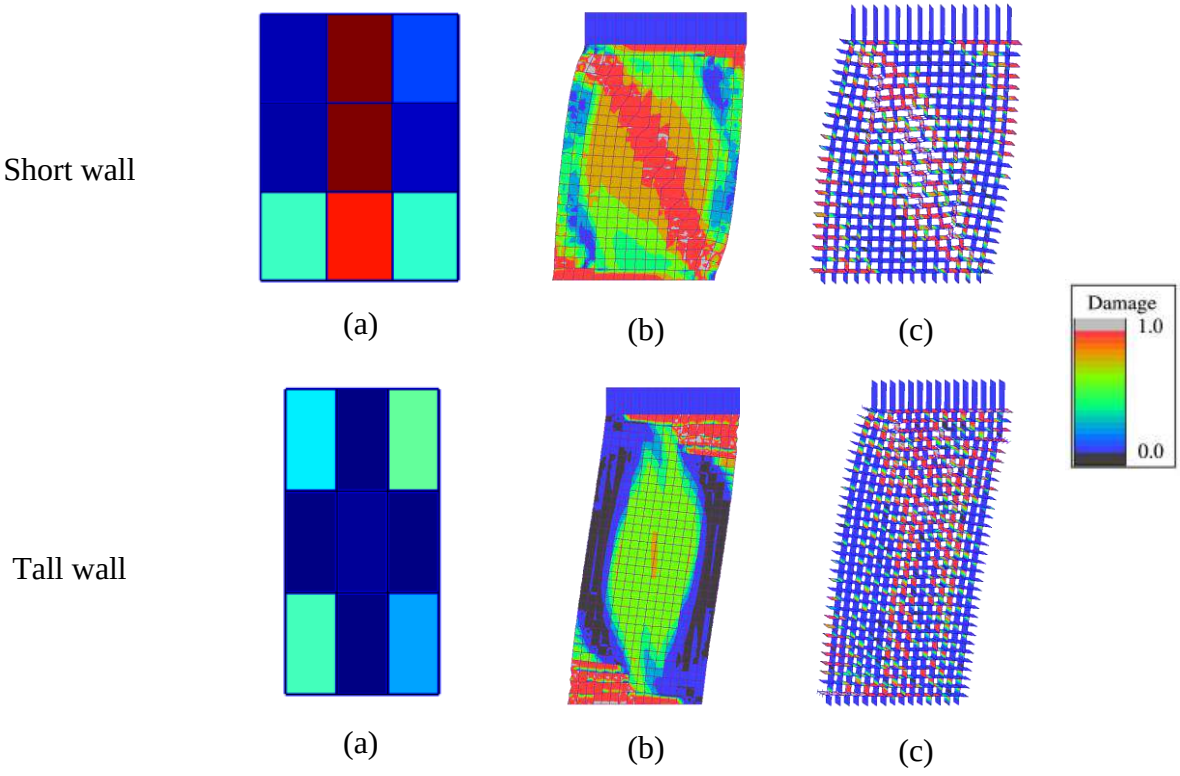


Figure 1. Damage patterns for two masonry walls predicted by (a) macroelement, (b) continuum macroscale and (c) mesoscale models.

References

[1] L. Macorini, B.A. Izzuddin, 2011, “A non-linear interface element for 3D mesoscale analysis of brick-masonry structures, International Journal for Numerical Methods in Engineering, Vol: 85, pages: 1584-1608.

[2] C. Chisari, L. Macorini, B.A. Izzuddin, 2020, “Multiscale model calibration by inverse analysis for nonlinear simulation of masonry structures under earthquake loading”, International Journal for Multiscale Computational Engineering, Vol. 18(2), pages: 241-263.

[3] E. Minga, L. Macorini, B.A. Izzuddin, I. Calio', 2020, "3D macroelement approach for nonlinear FE analysis of URM components subjected to in-plane and out-of-plane cyclic loading”, Engineering Structures, Vol. 220, 110951.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Preliminary Seismic fragility analysis of a URM building typology in Faial Island - Azores

Vasco Bernardo*, Shaghayegh Karimzadeh*, Daniel Caicedo*, Paulo B. Lourenço*

* ISISE, Department of Civil Engineering
University of Minho
Guimarães, Portugal
e-mail: vbernardo@civil.uminho.pt

Abstract: Masonry structures are extremely vulnerable to seismic events affecting the development of many countries worldwide. This study focuses on the seismic behaviour of a traditional masonry structure located in Faial Island – Azores (Portugal), which was hit by an earthquake of Mw = 6.2 on July 9th, 1998. The analyses were conducted through a probabilistic performance-based seismic approach employing a stochastic finite-fault ground motion simulation method to derive region-specific records and nonlinear numerical models to compute the capacity of the building. Subsequently, fragility curves are derived considering different seismic scenarios. The results show a significant probability of the structure reaching moderate to extensive damage.

Keywords: masonry structures, Faial Island (Azores), seismic fragility curves, seismic assessment

1. Introduction

In 1998, an earthquake of estimated Mw=6.2 hit Faial Island in the Azores, affecting the building stock and causing several structural damages. The traditional buildings in the Azores are mainly made of rubble stone masonry walls and flexible timber floors, which makes them highly vulnerable to seismic ground motions. This study derived seismic analytical fragility curves considering a representative building typology of Faial Island subjected to different seismic scenarios simulated through the stochastic finite-fault simulation method.

2. Seismic action modelling

The region-specific earthquakes are generated through the stochastic finite-fault ground motion simulation approach [1]. Simulations are performed on the bedrock for scenario events of different magnitudes through rupturing all active faults in the Island. Next, 6 alternative sets of records are selected from the database of scenario events with Mw of 5.0, 5.1, 5.2, 5.8, 6.0, and 6.2. Each set includes 10 records which satisfies the dispersion in terms of peak ground acceleration for each scenario earthquake.

3. Structural capacity and seismic response

3.1. Numerical modelling

A representative URM building typology of Azores with three stories high and rectangular plan (8.0 m x 12.6 m) is used for the subsequent analysis. A tridimensional numerical model is developed using an equivalent frame modelling strategy where the capacity is only governed by the in-plane behaviour. Details regarding the modelling assumption and material properties can be found in [2].

3.1. Seismic performance

Seismic performance is estimated using the improved Capacity Spectrum Method [3]. The capacity curve is computed using nonlinear static analyses with a load pattern proportional to the damage (adaptive pushover). The seismic demand is obtained for the different response spectrum, and the nonlinear response dispersion is computed.

4. Seismic fragility analysis

A log-normal cumulative distribution defines seismic fragility curves presented in Figure 1. These curves describe the probability of reaching or exceeding a given damage state (DS_1 – slight, DS_2 – moderate, DS_3 – severe, DS_4 – extensive) for a certain level of seismic intensity measure, expressed in this work as a function of spectral displacement. The following dispersion is considered [2]: $\beta c = 0.30$ and $\beta_{DSi} = 0.50$.

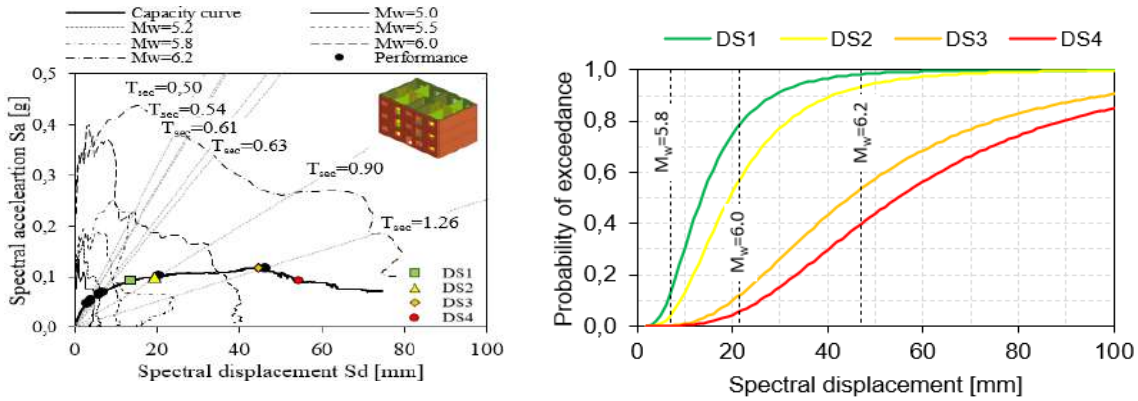


Figure 1. Seismic performance and fragility curves at bedrock.

5. Conclusions

Results show a significant probability that the structure will suffer moderate to extensive damage for a scenario of Mw=6.0 and Mw=6.2. Further analysis will be carried out on different typologies and other scenarios and considering the soil amplification at the surface.

Acknowledgements

This study was funded by the STAND4HERITAGE (ERC Grant agreement No. 833123).

References

[1] Assatourians, K., Atkinson, G. (2012). EXSIM12: a stochastic Finite-Fault Computer Program in Fortran, https://www.seismotoolbox.ca/EXSIM12.html (Last accessed 13 August, 2021).

[3] V. Bernardo, A. Campos Costa, P. Candeias, and A. Costa, "Seismic Vulnerability Assessment and Fragility Analysis of Pre-code Masonry Buildings in Portugal (under review - BEEE-D-21-00264R2)," *Bull. Earthq. Eng.*, 2021.

[3] FEMA, "Improvement of Nonlinear Static Seismic Analysis Procedures," *FEMA 440, Fed. Emerg. Manag. Agency, Washingt. DC*, 2005.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modelling of Connection Failure in Seismic Assessment of Masonry Structures

Fusco Daniela[*], Messali Francesco[†], Rots G. Jan[†], Addessi Daniela[*] and Pampanin Stefano[*]

[*] Dipartimento di Ingegneria Strutturale e Geotecnica (DISG)
Facoltà di Ingegneria Civile e Industriale, Sapienza Università di Roma
Rome, Italy
e-mail: daniela.fusco@uniroma1.it ; daniela.addessi@uniroma1.it; stefano.pampanin@uniroma1.it

[†] Department 3MD
Delft University of Technology
Delft, the Netherlands
e-mail: F.Messali@tudelft.nl; J.G.Rots@tudelft.nl

Abstract: In recent years, numerical modelling is increasingly being used to assess the seismic capacity of masonry buildings. In numerical models, the connections between structural walls are commonly considered as rigid, but in some cases this assumption may be inaccurate. Especially, this research focuses on the terraced houses built in the Netherlands after 1980s which are characterized by vertical glued joints between transverse masonry walls. Since the premature shear failure of these connections may cause a significant reduction of seismic capacity of the entire structures, different numerical approaches to represent the nonlinear behaviour of the joint are investigated and compared. The results of this work show that the strength of the vertical connection strongly affects the capacity of the structure, and the choice of constitutive law plays a crucial role in the robustness and accuracy of the model. In addition, a comparison between the numerical and experimental results is presented and discussed.

Keywords: continuous joints, seismic capacity, unreinforced masonry, numerical model, terraced house

1. Introduction

The Dutch terraced houses built after the 1980s are usually characterized by the use of large calcium silicate elements connected by thin layer mortar vertical joints with horizontal steel ties. The occurrence of the sliding shear failure of these connections may lead to a reduction of the seismic capacity of the building. For this reason it is essential to consider the nonlinear behaviour of the joint in the finite element model of the entire structure.

Several methods were developed to model the behaviour of masonry structures under seismic load. One of the most used approaches is the finite element method, where the behaviour of the masonry and joints is modelled through the nonlinear constitutive laws assigned to the elements. This work introduces two different smeared crack models adopted to describe masonry, the Total Strain Crack Model (TSCM) and the Engineering Masonry Model (EMM), comparing the results of the nonlinear analysis to the experimental results of one of two full-scale masonry assemblages tested in 2015 [1].

The modelling of the joint behaviour is discussed showing the advantages and disadvantages of using a constitutive law based on the Coulomb friction law or an uncoupled normal-shear relation. Several nonlinear analyses were conducted in order to compare the different modelling approaches to the experimental results both for a U-shaped element and for a masonry assemblage [2,3].

2. Results and Discussion

Nonlinear analyses at structural level were performed modelling one of two full-scale masonry assemblages tested at TU Delft in 2015 [1]. The results show that the use of different constitutive laws (TSCM and EMM) for masonry may predict different failure mechanisms of the structure [2,3].

In order to investigate the effect of the constitutive law of the vertical joint, Figure 1 shows the pushover response curves of a U-shaped element adopting the Coulomb friction model or the Nonlinear Elastic model, which decouples the force-displacement behaviour in the normal and tangential directions. The former represents the real nonlinear behaviour, but it leads to the numerical divergence of the analysis, whereas the latter provide more robust results but requires a careful calibration of the parameters. This result is also achieved at the structural level, introducing the vertical interface between the pier and the transverse wall in the masonry assemblage model previously mentioned [2,3].

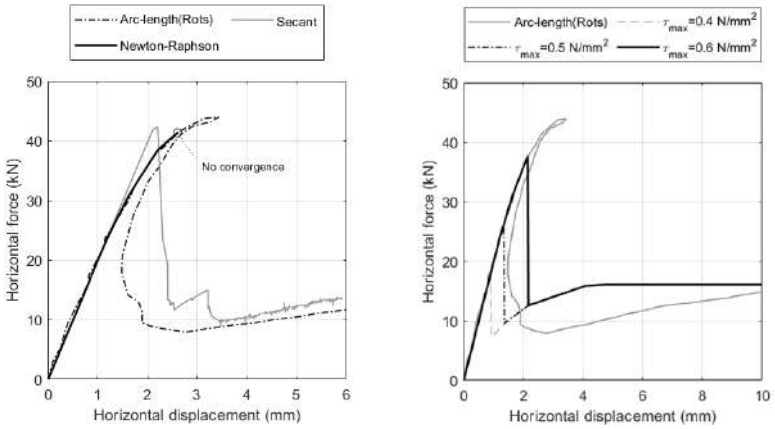


Figure 1. Capacity curves considering two different constitutive laws for connection: Coulomb Friction Model (left) and Nonlinear Elastic Model (right) [2]

4. Conclusions

The shear failure of the vertical connections in terraced house built after 1980s may reduce the seismic capacity of the structure. In nonlinear analysis model, the choice of the constitutive law for these connections is crucial to obtain robust and accurate results.

References

[1] Esposito, R., Terwel, K., Ravenshorst, G., Schipper, R., Messali, F., and Rots, J. 2017. Cyclic pushover test on an unreinforced masonry structure reseambling a typical Dutch terraced house. In 16th World Conference on Earthquake Engineering, Santiago, Chile.

[2] Fusco, D., F. Messali, J. Rots, D. Addessi, and S. Pampanin. 2021. Numerical study of pier-wall connections in typical Dutch URM buildings. In 12th International Conference on Structural Analysis of Historical Constructions: SAHC 2021. 2217–28.

[3] Fusco, D., F. Messali, J. Rots, D. Addessi, and S. Pampanin. 2022.Numerical issues on brittle shear failure of pier-wall continuous vertical joints in URM Dutch buildings. Engineering Structures 258:114078.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Tuning the failure of topologically interlocked structures

Koureas Ioannis, Pundir Mohit, Feldfogel Shai, David S. Kammer

Department of Civil Engineering (D-BAUG)
ETH Zurich
Zurich, Switzerland
e-mail: ikoureas@ethz.ch

Abstract: Topologically interlocked structures (TIS) are a promising class of engineering structures made of tunable building blocks. The mechanical response of TIS has been reported to outperform the monolithic equivalents in terms of ultimate strength, toughness and deformation. The interfacial interactions between the blocks and specifically the stick and slip mechanisms and the transition from one mechanism to the other are responsible for the highly non linear behavior in TIS. In this study, we employ the finite element method to analyze the effect of interface mechanisms on the load carrying capacity of beam-like TIS. Finite strain formulation is used to account for large rotation of the building blocks and is coupled with a node-to-segment contact algorithm (using penalty-based approach) to correctly enforce normal and tangential contact constraints along the interfaces. A parametric analysis is performed to understand the effect of friction coefficient, Young's modulus and the geometry of the blocks on the mechanical performance of the structure. We explain how these parameters control the stick and slip mechanisms and consequently the failure of the structure. We observe that the combination of interface mechanisms and geometry of the blocks provides an upper bound to the maximum load-carrying capacity of a structure.

Keywords: Architectured Structures, Frictional Contact, Hierarchical Interfaces

1 Introduction

Topologically interlocked structures (TIS) are developed using unbonded building blocks that interact with each other through contact. The interlocking nature of TIS provides resistance against failure. When the structure is loaded, the blocks can stick, slip and rotate with respect to each other (here we refer to stick, slip and rotation as TIS's mechanisms). The material and geometrical properties of these blocks can be adjusted, and therefore the toughness and strength of the structure can be tuned. However, the effect of TIS's mechanisms on the load-carrying capacity and the mechanical response of the structure is not fully understood. Here, we aim to provide a fundamental understanding on the effect of material properties (i.e., Young's modulus E and friction coefficient μ) and geometrical properties (i.e., height h of the blocks and hierarchical interface modifications) to the load-carrying capacity of beam-like TIS.

2 Results

In this study we address the effects of E, μ, h and interface geometry on the response capacity of beam-like TIS, using a finite element solver that accounts for large rotations and large deformations coupled with a node-to-segment frictional contact algorithm, with penalty-based constraints [1]. From our analysis of beam-like structures with planar interfaces we

observe that by increasing μ, the load-carrying capacity increases up to a maximum limit while sticking mechanism is promoted [2]. h has no significant effect on the load-carrying capacity. However, by increasing h, sliding is promoted. Finally, E scales linearly with the load-carrying capacity and it does not affect the mechanisms of the structure [2]. By modifying the interface geometry of the blocks using hierarchical interlocking we can reach the upper limit in the load-carrying capacity of TIS using realistic friction coefficients [3].

3 Conclusions

In this study, we analyse the effect of material and geometric parameters on the mechanisms (i.e., stick, slip and rotation) and the response capacity of beam-like topologically interlocked structures (TIS). Our findings show that beam-like TIS have an upper bound in the load-carrying capacity which can be achieved by increasing the friction coefficient of the structure or by modifying the interface geometry of the blocks. The latter is preferable since it allows to reach the upper limit using lower and more realistic friction coefficient values. The insights from this study, can be helpful in understanding how to choose the appropriate parameters for designing high performance TIS.

References

[1] Vladislav A. Yastrebov. *Numerical Methods in Contact Mechanics*. John Wiley & Sons, Inc., Hoboken, NJ USA, 2013. doi: 10.1002/9781118647974.

[2] Ioannis Koureas, Mohit Pundir, Shai Feldfogel, and David S Kammer. On the failure of beam-like topologically interlocked structures. *International Journal of Solids and Structures*, 259:112029, 2022. doi: https://doi.org/10.1016/j.ijsolstr.2022.112029.

[3] Ioannis Koureas, Mohit Pundir, Shai Feldfogel, and David S. Kammer. Beam-like topologically interlocked structures with hierarchical interlocking, 2022. URL `https://arxiv.org/abs/2212.06454`.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

The effects of material properties on the behavior and the failure of Topologically Interlocked Structures

Feldfogel Shai[*], Karapiperis Konstantinos[†], Andrade Jose[°], and Kammer, David S.[*]

[*] Dept. of Civil, Environmental and Geomatic Engineering (BAUG)
ETH Zurich
Zurich, Switzerland
e-mail: sfeldfogel@ethz.ch, dkammer@ethz.ch

[†] Department of Mechanical and Process Engineering (DMAVT)
ETH Zurich
Zurich, Switzerland
e-mail: kkarapiperis@ethz.ch

[°] Department of Mechanical and Civil Engineering
Caltech
Pasadena, California, USA
e-mail: jandrade@caltech.edu

Abstract: Topological Interlocking Structures (TIS) are discrete structural assemblies made of specially-shaped and un-bonded building blocks which hold together due to their interlocking geometries. TIS have been increasingly explored in the past twenty years, and their unique structural properties have been repeatedly observed in experiments. However, some fundamental aspects of the behavior have not yet been clarified, likely due to the challenge of capturing their contact-governed behavior and failure using conventional numerical models. Specifically, the effects of Young's modulus and the friction coefficient on the carrying capacity and the failure mechanisms of TIS assemblies slabs have not been systematically addressed and remain unclear. Here we address this fundamental question aspects through a numerical parametric study of centrally loaded slabs - the most common TIS application. Our study is based on the Level-Set-discrete-Element-Method, a recently developed approach capable of handling the multiple contact and friction interactions that govern the response of TIS. We find that the carrying capacity and structural stiffness scale linearly with Young's modulus, and that they reach a saturated limit for high values of the friction coefficient. We further find that the saturated response defines an upper-bound on the capacity of experimentally tested slabs.

Keywords: Topologically Interlocked Structures, Topologically Interlocked Materials, DEM

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Nonlinear analysis of masonry structures reinforced with the CAM system

Di Re Paolo, Greco Mattia and Lofrano Egidio

Department of Structural and Geotechnical Engineering
Sapienza University of Rome
Rome, Italy
e-mail: paolo.dire@uniroma1.it, ing.mgreco@outlook.it, egidio.lofrano@uniroma1.it

Abstract: This work focuses on the numerical analysis of masonry elements reinforced with the CAM system. An efficient macromechanical finite element modeling approach is proposed to reproduce the nonlinear response of such structures, based on a plastic-damage material model. Three main factors are investigated: setting of the steel stripes pre-tensioning values, definition of the boundary conditions, and calibration of the stripes post-yielding behavior. Hence, sensitivity analyses on pretensioning stress are carried out to investigate the effectiveness of the CAM system and provide designers with some useful recommendation.

Keywords: Reinforced Masonry, CAM System, Experiments, Finite Element Method, Plasticity, Damage

1 Introduction

Masonry structures are an important part of the European architectural heritage. Evaluation and protection of these compounds remain a difficult task because of the effects induced by low tensile strength and poor ductility. This work focuses on finite element (FE) modeling of structural elements reinforced by the CAM system, introduced by Marnetto and Dolce in 1999 [1]. The reinforcing CAM system is based on the introduction of a reticulum of steel stripes that extend in the vertical and horizontal directions and connect the two faces of a wall (Figure 1(a)). These aim to improve the structural performance of the masonry and create or restore effective connections among the elements.

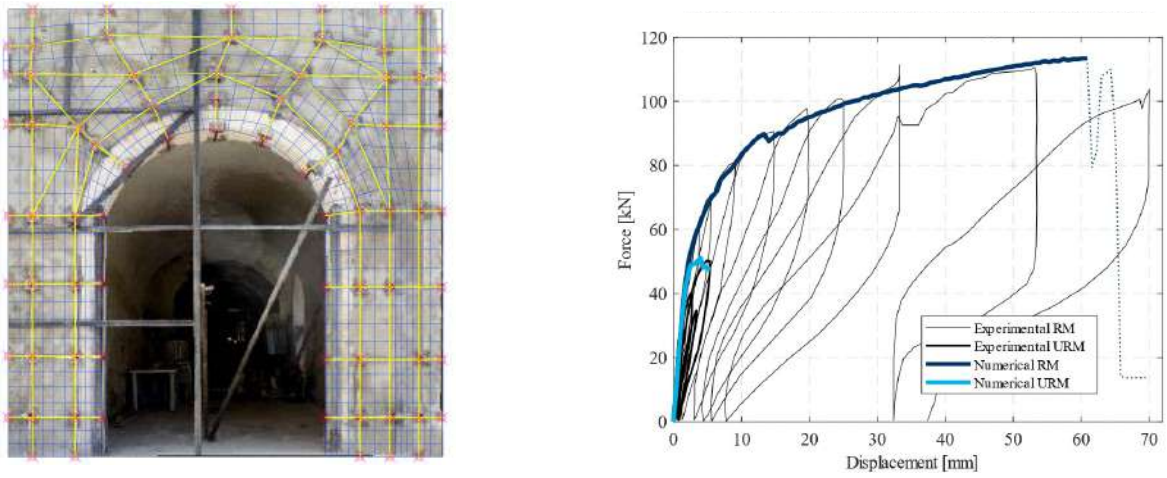
2 Modeling approach and numerical tests

To simulate the response of such structures, a FE macromodeling approach is proposed [2] where masonry is described using solid or plane FE, while stripes are considered as elasto-plastic truss elements that work only in tension (Figure 1(a)). A three-dimensional plastic damage constitutive law is adopted for masonry. This couples an isotropic two-variable damage model with the Drucker-Prager plasticity formulation.

Uniaxial stress analyses are conducted to investigate the performance of the material model in representing the behavior of representative volume elements of reinforced masonry. Moreover, specific relationships are proposed to define the damage threshold parameters from the plastic ones and avoid convergence issues in the solution procedure.

The response of a full-scale masonry arch wall experimentally tested by Spinella et al. [3] is numerically reproduced by adopting the proposed modeling approach (Figure 1). Sensitivity

analyses of pretensioning stress and post-yielding behavior are carried out to investigate the effectiveness of the CAM system and provide designers with some useful recommendations.



(a) (b)

Figure 1: Masonry arch wall: (a) superimposition of the FE mesh on the masonry specimen and (b) comparison of the experimental and numerical results in terms of global response curves

3 Conclusions

The analyses show that, for an accurate description of the structural response, the post-yielding behavior of the stripes must be calibrated correctly, as opposed to the pretensioning stress, whose effect is marginal. Moreover, the definition of the boundary conditions may have an impact on the effectiveness of the global solution.

4 Acknowledgements

P. Di Re and M. Greco acknowledge the research grant from Sapienza University of Rome, SEED PNR 2021 - 000048_21_SEED_DI_RE - CUP B89J21032850001.

References

[1] Dolce M, Cacosso A, Ponzo FC, Marnetto R. New technologies for the structural rehabilitation of masonry constructions: concept, experimental validation and application of the CAM system. Proceeding of: The intervention on built heritage: conservation and rehabilitation practices. Porto. 2002

[2] Di Re P, Greco M, Lofrano E, Paolone A. Finite element modeling of masonry elements reinforced with the CAM system. Structures 2022; 44:740-754.

[3] Spinella N, Colajanni P, Recupero A. Experimental in situ behaviour of unreinforced masonry elements retrofitted by pre-tensioned stainless-steel ribbons. Constr Build Mat 2014; 73: 740-53

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

An adaptive virtual element approach to upper bound limit analysis of cracked structures

Chiozzi Andrea[*] and Grillanda Nicola[†]

[*] Department of Environmental and Prevention Sciences (DiSAP)
University of Ferrara
Ferrara, Italy
e-mail: andrea.chiozzi@unife.it

[†] Department of Civil and Structural Engineering (DEC)
University of Sheffield
Sheffield, UK
e-mail: n.grillanda@sheffield.ac.uk

Abstract: We present a novel adaptive virtual element scheme for the kinematic limit analysis of cracked structures, which allows to elegantly overcome some of the complexities associated to standard finite element strategies. The virtual element method (VEM) is a stabilized Galerkin formulation on arbitrary polytopal meshes, wherein the basis functions are implicit (virtual) — they are not known explicitly nor do they need to be computed within the problem domain. Suitable projection operators are used to approximate the bilinear form on each element into two parts: a first term that reproduces polynomial consistency and a correction term that ensures stability. The key idea is to exploit the main features of a second order VEM to naturally deal with a general mesh refinement algorithm based on a conforming polytree mesh structure, while avoiding volumetric locking. The method is well suited for arbitrary polygonal elements as well as traditional triangular and quadrilateral ones, considered as special cases. We here restrict the treatment to plane-strain limit analysis for von Mises-type materials, although its extension to other materials is straightforward. The adaptive mesh refinement scheme is guided by a strain rate indicator based on the L2-norm. Numerical experiments are performed, that illustrate for the proposed method a good accuracy and a low computational burden, allowing us to tackle large-scale limit analysis problems.

Keywords: virtual element method, limit analysis, adaptive mesh refinement, polytree mesh

1. Introduction

Limit analysis plays a major role in the context of elastic–plastic fracture and fracture-safe design. Adaptive finite element approaches to limit analysis have been widely investigated in the literature [1] and sophisticated mesh-refinement schemes have been consequently devised, with the aim of suitably refine the mesh in the regions of the problem domain where high plastic deformation concentrates [2-3]. Mesh-refinement algorithms must be guided by adequate error-based indicators. To this end, a multitude of indicators have been proposed in the last two decades, such as those based on a-posteriori error estimates [2-3] and dissipation-based indicators [4]. In addition, the conception of an automatic refinement mesh generator within the standard finite element framework is far from trivial and entails the occurence of hanging nodes, which need to be systematically dealt with, even in the cases using a quadtree data structure [5]. Recently, polygonal finite elements have been shown to provide greater flexibility for problems requiring automatic mesh refinement [6], particularly, in the field of limit analysis [7]. However, the implementation of polygonal finite elements is generally cumbersome and, furthermore, lowest-order displacement-based finite elements are known to poorly perform under incompressibility assumptions, so much

to require special enhancements, such as discontinuous enrichments of the velocity field [8] and bubble function enrichments [9].

2. Higher-order VEM-based adaptive limit analysis

In this contribution, we propose to overcome the aforementioned difficulties by introducing a second order virtual element approach for the adaptive limit analysis of cracked structures on polytree meshes. The Virtual Element Method (VEM) [10], is a stabilized Galerkin formulation on arbitrary polytopal meshes, wherein the basis functions are implicit (virtual) — they are not known explicitly nor do they need to be computed within the problem domain. The VEM is capable of naturally dealing with the presence of hanging nodes, while requiring minimum additional burden when it comes to higher order formulations, which, on the other hand, constitute a promising route to alleviate volumetric locking issues. The adaptive mesh refinement scheme is guided by a strain rate indicator based on the L2-norm [7]. Numerical experiments are performed, which illustrate for the proposed method a good accuracy, allowing the tackling of large-scale limit analysis problems.

References

[1] Christiansen E, Andersen KD. Computation of collapse states with von Mises type yield condition. Internat J Numer Methods Engrg 1999; 46:1185-1202.

[2] Borges LA, Feijoo RA, Zouain N. A directional error estimator for adaptive limit analysis. Mech Res Comm 1999; 26:555-563.

[3] Borges LA, Zouain N, Costa C, Feijoo R. An adaptive approach to limit analysis. Internat. J. Solids Structures 2001; 38:1707-1720.

[4] Martin CM. The use of adaptive finite-element limit analysis to reveal slip-line fields. Geotech Lett 2011; 1:23-29.

[5] Tabarrei A, Sukumar N. Adaptive computations on conforming quadtree meshes. Finite elem Anal Des 2005; 41:686-702.

[6] Spring DW, Leon SE, Paulino GH. Unstructured polygonal meshes with adaptive refinement for the numerical simulation of dynamic cohesive fracture. Int J Fract 2014; 189:33-57.

[7] Nguyen-Xuan H, Nguyen-Hoang S, Rabczuk T, Hackl K. A polytree-based adaptive approach to limit analysis of cracked structures. Comput Methods Appl Mech Engrg 2017; 313:1006-1039;

[8] Sloan SW, Kleeman PW. Upper bound limit analysis using discontinuous velocity fields. Comput Methods Appl Mech Engrg 1995; 127:293-314.

[9] Nguyen-Xuan H, Liu GR. An edge-based finite element method (ES-FEM) with adaptive scaled-bubble functions for plane strain limit analysis. Comput Methods Appl Mech Engrg 2015; 285:877-905.

[10] Beirão da Veiga L, Brezzi F, Cangiani A, Manzini G, Marini LD, Russo A. Basic principles of virtual element methods. Math Models Methods Appl Sci 2013; 23:199-214.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Analysis of out-of-plane loaded masonry walls via discontinuity layout optimization

Grillanda, Nicola*, He, Linwei* and Gilbert, Matthew*

* Department of Civil and Structural Engineering,
University of Sheffield, Mappin Street, Sheffield S1 3JD, UK
e-mail: n.grillanda@sheffield.ac.uk, linwei.he@sheffield.ac.uk, m.gilbert@sheffield.ac.uk

Abstract: An upper bound limit analysis formulation based on the discontinuity layout optimization (DLO) procedure is proposed for determining the out-of-plane resistance of masonry walls. With DLO the model is discretized using nodes that are interconnected by potential yield-lines, along which the main variables of the kinematic problem are defined. The internal energy dissipation is quantified by considering the mechanical properties of the masonry material employed. Once the required constraints are defined, a linear programming problem can be solved to find the critical yield-line pattern and the associated collapse load factor.

Keywords: discontinuity layout optimization, limit analysis, masonry panels, out-of-plane failure.

1. INTRODUCTION

Masonry walls have been widely used as principal structural elements in load bearing masonry structures and also as secondary elements in steel and concrete framed structures. Thus, the analysis of their collapse behaviour is still a topic of interest. Although historic masonry is usually assumed to possess no-tensile resistance at joints [1], in modern masonry construction some flexural tensile capacity is usually assumed. This has led to the yield-line method being used to determine the capacity of out-of-plane loaded masonry walls [2]. To systematically automate the yield-line method the Discontinuity Layout Optimization (DLO) has been proposed for the analysis of concrete slabs [3,4]. However, its application to out-of-plane loaded masonry walls has still to be investigated. Here a simple DLO-based formulation is proposed for the out-of-plane analysis of masonry walls.

2. DLO FORMULATION

Given an external reference system *Oxyz*, consider a masonry wall on the *xy* plane in which *y* is the vertical axis. The DLO analysis requires discretization of the wall into nodes connected via potential yield-lines, at which displacement jumps can occur; these displacement jumps constitute the main variables in the problem. If we denote as *n* and *s* respectively the normal and the tangential axes for a given yield-line, the main variables include the rotations θ_n and θ_s and the displacement δ_z for out-of-plane plasticity problems. The resulting linear programming (LP) problem can be written as follows:

$$\min \lambda \mathbf{f}_L^T \mathbf{d} = -\mathbf{f}_D^T \mathbf{d} + \mathbf{g}^T \mathbf{p} \text{ subject to} \begin{cases} \mathbf{B}\mathbf{d} = \mathbf{0} \\ \mathbf{N}\mathbf{p} - \mathbf{d} = \mathbf{0} \\ \mathbf{f}_L^T \mathbf{d} = 1 \\ \mathbf{p} \geq \mathbf{0} \end{cases} \quad (1)$$

where λ is a live-load multiplier, $\mathbf{f}_L$ and $\mathbf{f}_D$ represent live and dead loads, $\mathbf{d}$ and $\mathbf{p}$ are vectors containing respectively displacement and the non-negative plastic multiplier variables, $\mathbf{g}$ is a vector used to evaluate the internal energy dissipation, $\mathbf{B}$ is the compatibility matrix, and $\mathbf{N}$ is the matrix defining the plastic flow. For slender walls, it is reasonable to assume that

collapse occurs due to rotations along hinge lines, where the generalized plastic bending moment can be assumed as:

$$m_p^x = \frac{(f_x + \sigma_y)t^2}{6};\ m_p^y = \frac{f_y t^2}{6}\ ;\ m_p^\phi = m_p^x \cos\phi^2 + m_p^y \sin\phi^2 \quad (2)$$

where f_x and f_y represents the flexural tensile strength values along the *xz* and *yz* planes respectively, σ_y is the vertical stress deriving from permanent loads, t is the thickness and ϕ is the inclination of the line.

3. SIMPLE FULL PANEL

Originally presented in [5], a simple masonry panel subjected to uniform out-of-plane pressure is presented as the first example in the present study. The panel has area 5000×2800 mm^2 and thickness 150 mm. All the edges are simply supported and no in-plane actions are considered here (as assumed in [5]). $f_x = 0.94$ N/mm^2 and $f_y = 0.32$ N/mm^2 have been assigned as flexural tensile strengths. The yield-line pattern derived via DLO is presented in Figure 1; this is in good agreement with the typical response of out-of-plane loaded panels. The corresponding pressure at failure is equal to 5.23 kN/m^2, which is slightly lower than the value of 6.6 kN/m^2 obtained via an anisotropic finite element model in [5].

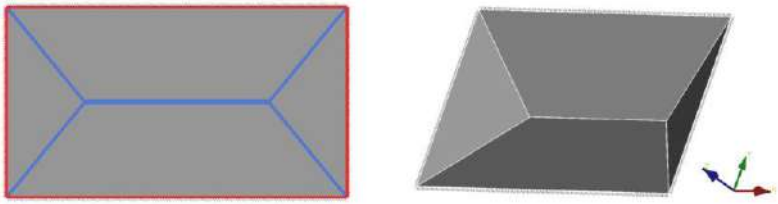


Figure 1. Simply supported full panel under uniform out-of-plane pressure, yield-line pattern found via DLO (red and blue lines denote hinge lines with cracks opening on the front and the rear faces respectively) and corresponding mechanism.

4. CONCLUSIONS

The presented DLO formulation appears well-suited for the efficient evaluation of the out-of-plane capacity of masonry wall panels. The procedure allows the critical yield-line pattern to be determined directly, without the need to implement complex mesh adaptation strategies, which can be time-consuming and unreliable. Other numerical examples will be studied and in future the procedure can be extended by using homogenization strategies to determine internal energy dissipation functions relevant to historic masonry walls.

REFERENCES

[1] Heyman J. The stone skeleton. Int J Solids Struct 1966;2:249-279.

[2] EN-1996-1-1:2019 Eurocode 6. Design of masonry structures. Part 1-1: General rules for reinforced and unreinforced masonry structures.

[3] Gilbert M, He L, Smith CC, Le CV. Automatic yield-line analysis of slabs using discontinuity layout optimization. Proc R Soc A. 2014;470(2168):20140071.

[4] He L, Gilbert M, Shepherd M. Automatic yield-line analysis of practical slab configurations via discontinuity layout optimization, J Struct Eng 2017;143(7):04017036.

[5] Lourenço PB. Anisotropic softening model for masonry plates and shells, J Struct Eng 2000;126(9):1008-1016.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Identifying Thrust Layouts in Masonry Gravity Structures

Nanayakkara, K. Isuru [†*], Liew, Andrew[†] and Gilbert, Matthew[†]

[†]Department of Civil and Structural Engineering,
the University of Sheffield,
Mappin Street, Sheffield S1 3JD
[*] e-mail: kiunanayakkara1@sheffield.ac.uk

Abstract: A new automated analysis procedure for masonry gravity structures, termed thrust layout optimization (TLO), is described. TLO has been designed to rapidly assess structural load-carrying capacity and to overcome limitations of the traditional thrust line analysis method. Making use of standard ground-structure layout optimization, thrust layouts are identified that are highly visual, allowing areas where tensile strength is implicitly assumed to be clearly identified; this is beyond the scope of the traditional thrust line analysis method. Also, sliding failures can be modelled without difficulty. The procedure is further extended to enable identification of the optimal locations of strengthening measures.

Keywords: limit analysis, masonry, thrust line, optimization

1 Introduction

A considerable proportion of existing building and other constructed infrastructure across the world comprises traditional masonry gravity structures. Masonry also has the potential to be more widely used in the future, taking advantage of low embodied carbon materials such as natural stone [1]. Although a wide range of analysis and design methods are available, ranging from thrust line analysis methods to non-linear finite element analysis (FEA) methods, the traditional thrust line analysis method has limitations [2], and non-linear FEA methods generally demand significant computational power and user expertise [3].

In this work, various limitations of the traditional thrust line method are addressed, with a new automated procedure capable of automatically identifying thrust layouts presented and then applied to various practical examples.

2 Thrust layout optimization (TLO)

Thrust lines—generated either via hanging chains or graphic statics—have been extensively used for the analysis and design of masonry gravity structures. However, it is implicitly assumed that a structure is made up of vertical strips, with the actual locations of masonry joints (the 'stereotomy') disregarded; this leads to inaccurate outcomes [2]. Furthermore, its treatment of the tensile strength of the material is often not transparent to users.

Thrust layouts are presented here that recognise actual block stereotomy and also the available, albeit usually limited, tensile capacity of masonry blocks. The thrust layouts identified improve upon the traditional thrust line analysis method by ensuring all individual blocks are in equilibrium, whilst also allowing visualization of the flow of forces through the structure.

Recognising the correspondence between graphic statics and ground-structure layout optimisation (LO), generation of thrust layouts is automated via a new procedure, termed thrust layout optimization (TLO). This involves a load-carrying capacity evaluation step followed by post-processing steps to visualise the corresponding flow of forces. Sliding at block interfaces can readily be modelled if required.

The thrust layouts identified via TLO provide a rich visual representation of the flow of forces in masonry gravity structures; forces flow naturally around internal holes, with blocks rocking about vertices leading to patterns of forces resembling classical Michell structures; more familiar funicular thrust lines can also be identified (Fig 1a). TLO can also be extended to determine the optimal (minimum volume) placement of strengthening measures in gravity masonry structures—see Fig 1b.

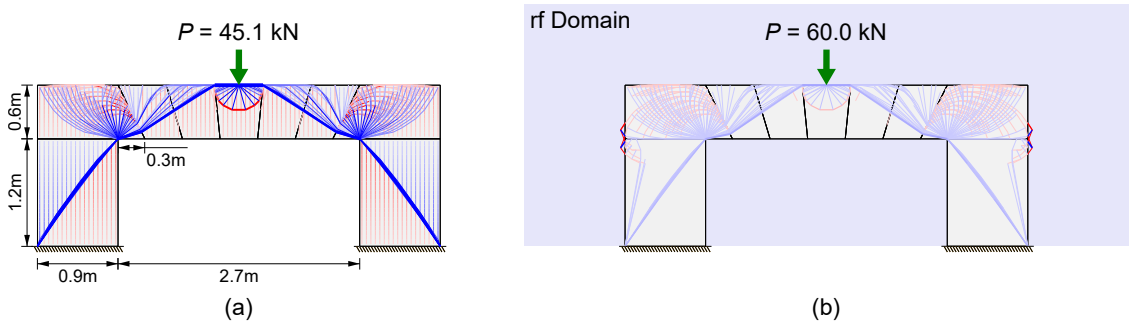


Figure 1: Flat arch on stone columns: (a) thrust layout at the collapse load (P of 45.1 kN); (b) optimal placement of external strengthening measures (at the left and right edges of the structure) to carry an increased load P of 60.0 kN (mobilization of self-weight also plotted in (a); lines in blue and red represent compressive and tensile forces respectively, with thickness corresponding to force magnitude; thrust layout shaded lighter in (b); geometry as indicated; material unit weight = 25 kN/m^3; width = 1 m).

3 Conclusions

A new procedure, termed thrust layout optimization (TLO) is presented to assess the collapse load of masonry gravity structures and to generate thrust layouts to visualise the flow of forces. Unlike the traditional thrust line method, the actual block stereotomy and tensile strength of the masonry are considered. It is also shown that the TLO method can be extended to determine the optimal placement of strengthening measures in masonry gravity structures.

References

[1] Webb S. Stone Rises. RIBA J. 2020;127:52–54.

[2] Heyman J. La Coupe des Pierres, in: Proceedings of the Third International Congress on Construction History. 2009; Cottbus, Germany.

[3] Roca P, Cervera M, Gariup G, Pela' L. Structural analysis of masonry historical constructions. Classical and advanced approaches. Arch Comput Method E, 2010; 17:299–325.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Parametric analysis of multi-ring arches

Nela Bledian[*,a], **Pingaro Marco**[*,b], **Reccia Emanuele**[†] **and Patrizia Trovalusci**[*,c]

[*] Department of Structural and Geotechnical Engineering (DISG)
Sapienza University of Rome
Rome, Italy
e-mail: [a]bledian.nela@uniroma1.it, [b]marco.pingaro@uniroma1.it, [c]patrizia.trovalusci@uniroma1.it

[†] Department of Civil and Environmental Engineering and Architecture
University of Cagliari
Cagliari, Italy
e-mail: emanuele.reccia@unica.it

Abstract: Among a majority of build heritage that cover large spans are constructed with curved masonry elements such multi-ring arches in order to achieve bigger overall thickness. The various methods of construction used for multi-ring arches have a significant impact on the outcome of their ultimate capacity to external actions. Since such structures consist of separate rings that interact through interface contacts, the disposition of the units and the internal mechanical parameters such as friction are of great influence. Furthermore, it is very evident that also geometrical characteristics play a major role on the behavior of such structures. A full combination of these parameters, namely, friction angle, disposition and size of blocks, number of rings and span, are considered in the assessment of multi-ring arches under the vertical load at quarter span utilizing an in-house code that follows the upper bound limit analysis approach. The significance of each parameter is shown after their combination of effects in terms of collapse multipliers that are categorized as per respective influencing parameters. It is shown that for various spans and different geometries, the interlocking effect from the disposition of units and the friction angle, influence the whole structural behavior.

Keywords: Multi-ring Arches, Ring Separation, Limit Analysis, Sliding Mechanism

1 Discussion and Results

One of the initial works in the field of multi-ring arches is that of Melbourne & Gilbert [1] where the importance of internal interaction between the blocks and their disposition was demonstrated. Additionally they show the differences in accounting for the internal structure of the rings and the different collapse mechanisms achieved. Recently, a parametric study is performed by Kassotakis *et al.* [2] where they study different spans and number of rings for the multi-ring arches using the Discrete Elements Method. This study intends to perform a parametric study on some key influential parameters involving a large data set. Using an improved in-house code from the original work of [3], that implements an upper bound limit analysis approach, multi-ring arches are studied. For the arches are considered three different spans (S) varying from $3.0m$, $5.0m$ and $7.0m$. The geometry of the arch consists of a various number of rings (R) of constant thickness (t) per ring, constructing in this way different overall thicknesses (T), varying from 1 to 5 rings. For each type of arch in terms of rings, an equivalent (EQ) thickness of one ring arch is analyzed as well. Two different sizes of blocks

(B) are chosen to construct the ring, namely, 33 blocks per ring and 99 blocks per ring to differentiate bigger and smaller blocks, respectively. The general texture for the disposition of voussoirs consists of stack and running bond with a parametrization of the interlocking (I) between blocks. Interlocking is represented with a coefficient of interlock (β - in percentage) relative to the thickness of the block (b) that varies from 0% (no interlock; stack), 15% and 35% (medium interlock; running) up to a maximum of 50% (complete interlock; running) as schematically shown in Fig.1(left). Finally the live load for the assessment is taken as vertical applied at the left quarter-span of the arch. Outcomes in terms of collapse multipliers for the span of $3m$ and two examples of collapse mechanisms are provided in Fig.1.

Acknowledgments
This work is supported by: Italian Ministry of University and Research PRIN 2017 (B88D19001130001, No.2017HFPKZY); Progetto Grande di Ateneo 2021 (CUP:B85F21008380001); Progetto Medio di Ateneo 2022.

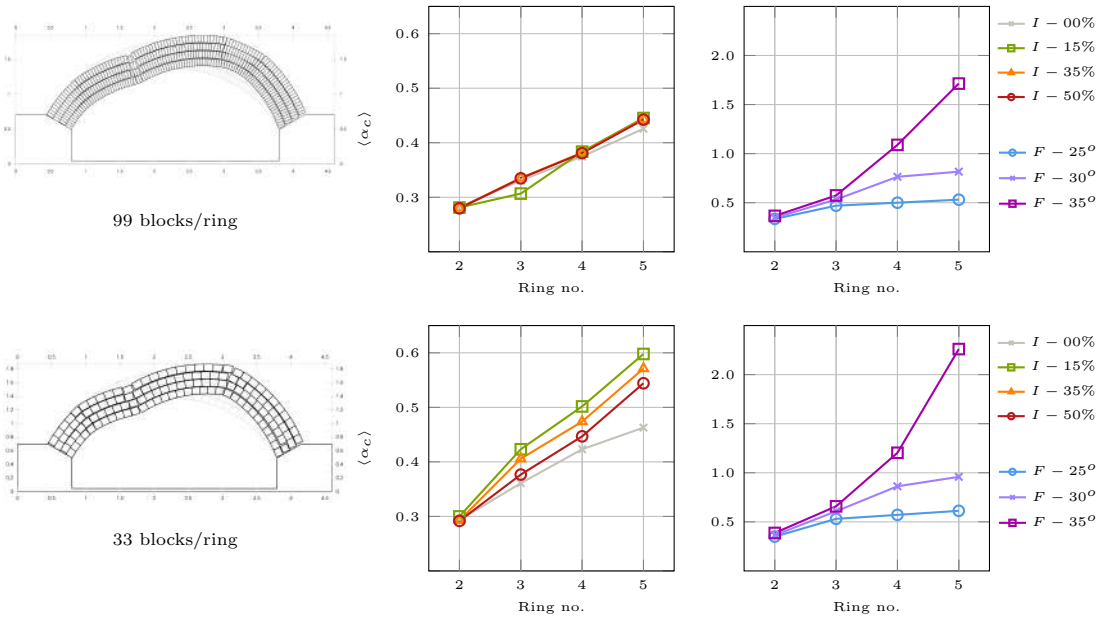


Figure 1: Influence of the interlocking percentage (I) and friction angle (F) on the collapse multipliers for the multi-ring arches made up of 2 to 5 rings. Results for the arches 99 blocks per ring (top graphs) and 33 blocks per ring (bottom graphs), and two examples of collapse mechanisms (Span $3m$; 4 Rings; 15% Interlock; 30^o Friction), with respective no. of blocks.

References

[1] Melbourne C, Gilbert M. The behaviour of multiring brickwork arch bridges. The Structural Engineer Vol.73 No.3 1995;39-47.

[2] Kassotakis N, Sarhosis V, Forgacs T, Bagi K. Discrete element modelling of multi-ring brickwork masonry arches. 13th Canad Mason Symp, Halifax, Canada; 2017.

[3] Baggio C, Trovalusci P. Collapse behaviour of three-dimensional brick-block systems using non-linear programming. Struct. Engineering and Mechanics, 10(2), 181–195; 2000.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Dynamic analysis of multi-block masonry structures under ground motion excitation

Nicola A. Nodargi and Paolo Bisegna

Department of Civil Engineering and Computer Science
University of Rome Tor Vergata
Rome, Italy
e-mail: {nodargi; bisegna}@uniroma2.it

Abstract: The dynamic analysis of multi-block masonry structures subjected to ground motion excitation is addressed. An event-driven computational approach is proposed, which exploits a novel variational formulation for describing both the regular motion of the structure and the impacts occurring between its blocks. The kinetic energy loss at impacts is determined by extending the Housner impact model originally proposed for the rocking motion of a single rigid block. For an insight into the impulsive stress state arising within the structure at impacts, the original concept of impulse line is proposed, which is analogous to the thrust line prevailing at regular instants of motion. From the computational standpoint, the solution of straightforward quadratic-programming problems is required for the dynamic analysis to advance in time. Numerical results are presented in comparison to competing computational strategies available in the literature.

Keywords: Masonry, Dynamic analysis, Rocking, Impact model, Multi-block arch

Arches are peculiar structural elements of historical masonry constructions, whose stability in seismic regions may be endangered by earthquakes. A common approach for a seismic safety assessment resorts to an equivalent static analysis based on the classical Heyman assumptions [1]. The minimum peak ground acceleration needed to transform the arch into a mechanism and initiate its motion is thus determined, providing a safe estimate of the arch vulnerability under a time-varying ground motion excitation.

The way towards the dynamic analysis of masonry arches subjected to ground acceleration was opened by Housner's seminal work on the rocking motion of a single rigid block. As consisting in the alternate rotation of the block about its bottom corners, that work derived the equation of motion prevailing at regular instants and the kinetic energy loss at impacts. The latter computation assumed that concentrated impulse forces are transmitted through the pivotal points of the block. Generalizing that contribution, a first dynamic analysis of a masonry arch was carried out by Oppenheim [3]. Basic assumption was that the arch moves along the four-hinge mechanism determined through an equivalent static analysis. Direct overturning was investigated as a possible failure condition of the descending single-degree-of-freedom system under an idealized ground motion pulse. In [4], De Lorenzis and coauthors extended Oppenheim's approach to address the rocking motion of masonry arches. That required adapting the Housner impact model, as conceived for a single rigid block, to an arch behaving as a four-hinge mechanism. The two assumptions were made that (i) the hinges after the impact are mirrored from those before the impact, and that (ii) the impulse forces at the hinge sections before the impact are located on the opposite side of the hinges across the arch thickness. As a result, it was shown that, depending on the ground impulse

shape, an arch may survive the first half cycle of motion, but overturn, after an impact is occurred, during the second half cycle. As noticed in [4], a possible shortcoming of that approach is that the thrust line may exit the thickness of the arch during the regular instants of motion, thus revealing the simplification inherent to the four-hinge mechanism assumption. In [5], the dynamic analysis of a masonry arch regarded as a system of rigid blocks has been undertaken, assuming that hinges may open and close, and impact may occur, at any joint between the blocks. A recent contribution [6] has re-considered the extension of the Housner impact model from the original case of a single rigid block to the more complicated case of masonry arch behaving as a single-degree-of-freedom system. By introducing the novel concept of impulse line at impact, which is analogous to the thrust line at regular instants of motion, the intuitive result that impulse forces need to be transmitted through the hinges opening after the impact has been demonstrated. Furthermore, the minimization of kinetic energy loss at impact has been proven as the condition governing the hinge locations after the impact and the static admissibility of the resultant impulse forces.

The dynamic analysis of multi-block masonry structures subjected to ground motion excitation is here addressed. An event-driven computational approach is proposed. It is based on a novel variational formulation, which describes both the regular motion and impacts, and amounts to the solution of straightforward quadratic-programming problems [7]. Numerical results are presented in comparison to competing computational strategies available in the literature (e.g., see [8, 9]).

References

[1] Heyman J. The stone skeleton. Cambridge University Press; 1995.

[2] Housner GW. The behavior of inverted pendulum structures during earthquakes. Bull Seismol Soc Amer 1963;53(2):403–417.

[3] Oppenheim IJ. The masonry arch as a four-link mechanism under base motion. Earthq Eng Struct Dyn 1992;21(11):1005–1017.

[4] De Lorenzis L, DeJong M, Ochsendorf J. Failure of masonry arches under impulse base motion. Earthq Eng Struct Dyn 2007;36(14):2119–2136.

[5] Kollár LP, Ther T. Numerical model and dynamic analysis of multi degree of freedom masonry arches. Earthq Eng Struct Dyn 2019;48(7):709–730.

[6] Bisegna P, Coccia S, Como M, Nodargi NA. Impacts analysis in the rocking of masonry arches. 2023; submitted.

[7] Nodargi NA, Bisegna P. Dynamic analysis of multi-block masonry structures under ground motion excitation. 2023; submitted.

[8] Krabbenhoft K, Lyamin AV, Huang J, Vicente da Silva M. Granular contact dynamics using mathematical programming methods. Comput Geo 2012;43:165–176.

[9] Portioli FPA. Rigid block modelling of historic masonry structures using mathematical programming: a unified formulation for non-linear time history, static pushover and limit equilibrium analysis. Bull Earthq Eng 2020;18:211–239.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Fracture in Polymers: Discrete-to-Continuum Coupling

Felix Weber[*,†], Christof Bauer[*,†], Maximilian Ries[†], Wuyang Zhao[†] and Sebastian Pfaller[†]

[*] Competence Unit for Scientific Computing (CSC)
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
Erlangen, Germany
e-mail: felix.w.weber@fau.de

[†] Institute of Applied Mechanics
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
Erlangen, Germany

Abstract: When it comes to fracture of polymers, intriguing phenomena take place at the molecular level of detail, whereas the boundary conditions are macroscopic in nature. However, the high computational cost of particle-based calculations makes the use of multiscale techniques indispensable. The Capriccio method is one such approach designed for amorphous polymers, which concurrently couples particle domains described by molecular dynamics (MD) and a continuum discretized by the finite element method (FEM). The domain coupling takes place in an overlapping region, whereby the MD domain is subjected to non-periodic, so-called stochastic boundary conditions (SBC). Our aim is to expand the capabilities of the Capriccio method to adaptive fracture and crack propagation simulations of polymeric materials. One crucial aspect is that molecular mechanisms related to fracture must be integrated into the MD framework in an appropriate way. Currently, we use a coarse-grained description for polystyrene as a sample system. Recent investigations in progress include replacing the harmonic potentials originally employed for the bonded interactions by formulations which are more appropriate for covering bond dissociation.

Keywords: Polymer fracture simulation, Particle-continuum coupling, Multiscale modelling, Molecular dynamics, Finite element method

1. Introduction

The Capriccio method [1] is a partitioned-domained simulation environment specifically designed for amorphous polymers. Specifically, particle regions governed by molecular dynamics (MD) are concurrently coupled to a continuum discretized by the finite element method (FEM). The MD and finite element (FE) regions overlap in a bridging domain, where the energy contributions of both descriptions are weighted. In the Capriccio method, the boundaries of the MD systems to be coupled to the continuum are subjected to non-periodic, so-called stochastic boundary conditions (SBC). Here, auxiliary particles, which we refer to as anchor points, are introduced, transferring the forces and displacements between the MD and FE regions. As an example system, we currently use a coarse-grained model for glassy polystyrene, which substitutes each chemical monomer by one superatom. The tabulated bonded, angle, and non-bonded potentials describing the interactions between the superatoms have been obtained by iterative Boltzmann inversion [2].

2. Multiscale fracture simulations using the Capriccio method

When it comes to investigations of the behavior of polymers during failure, insights into molecular mechanisms are of particular relevance. However, as soon as crack propagation in a classical fracture mechanical setup containing a preinduced crack (see Figure 1) is to be studied, periodic boundary conditions (PBC) are not sufficient. Instead, non-periodic MD systems are necessary to capture this type of pseudo-experimental setting. Furthermore, due

to the high computational cost inherent to MD simulations, multiscale approaches coupling MD to continuum descriptions are desirable. In [3], we have shown the suitability of the Capriccio method when it comes to MD-FE fracture simulations of glassy polymers. As a preliminary bond breakage criterion in the MD system, a specified cutoff for the harmonic bond potentials was applied. Current work in progress is to substitute the harmonic bond potentials by other potential formulations more reasonable in terms of bond breakage, for instance Morse potentials. Furthermore, the movement of the MD domain within the continuum according to the current crack tip position is envisaged. To this end, before switching from the FE to the MD description, the MD system is predeformed using a hybrid molecular dynamics-continuum mechanical approach [4], which accelerates the corresponding MD simulation. For switching back to FE, a displacement field is obtained from MD using the Murdoch-Hardy approach, which is then transferred to the FE domain.

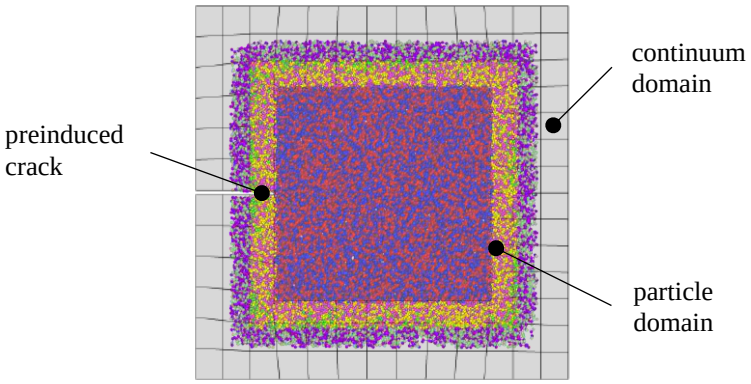


Figure 1. Setup of multiscale fracture simulations using the Capriccio method containing a preinduced crack. The given illustration is a cross section through a central plane.

4. Conclusions

In respect of fracture simulations of polymers, the multiscale Capriccio method is a promising environment in terms of both applying reasonable boundary conditions and keeping the computational cost to a minimum. Both our investigations on spatial adaptivity of the MD description according to the current crack tip position as well as on finding an potential formulation appropriate in view of bond dissociation contribute to its development to a powerful environment regarding the simulation of crack propagation pathways and the calculation of essential properties, for instance the fracture toughness.

References

[1] Pfaller S, Rahimi M, Possart G, Steinmann P, Müller-Plathe F, Böhm MC. An Arlequin-based method to couple molecular dynamics and finite element simulations of amorphous polymers and nanocomposites. Comput Methods Appl Mech Engrg 2013;260:109-129.

[2] Qian H, Carbone P, Chen X, Karimi-Varzaneh HA, Müller-Plathe F. Temperature-Transferable Coarse-Grained Potentials for Ethylbenzene. Polystyrene, and Their Mixtures. Macromolecules 2008;41:9919-9929.

[3] Zhao W, Pfaller S. A concurrent MD-FE coupling method towards simulations of fracture of thermoplastic polymers. Proceedings of XVI International Conference on Computational Plasticity. Fundamentals and Applications 2021;submitted manuscript.

[4] Bauer C, Ries M, Pfaller S. Accelerating molecular dynamics simulations by a hybrid moleculardynamics-continuum mechanical approach. Soft Mater 2022;20:428-443.

t ff b YYmk Uq w f Y
wfYA; AB
@ 8A@g A; AB7n 7n

c **c**

sb **c**

4 a Y 7
r s a 7
ECAGF a 7d
8 J 9 T 9 9 8 9

a Y 7
r s a 7
ECAGF a 7d

ü **s** U 7 2cb3
9m 7 2k a 3 8 7
7
9V 7
9 f 7 k a cb
8 8
9 f cb8k a 7
7k a
9 r 7
9k 7 8
f V f 2fVf3
8 9

s k 8 Ml 8 MY 8 Mf V
f 2fVf3

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A coarse-grained molecular dynamics model to analyze fracture in polymer nanocomposites

Maximilian Ries*, Vincent Dötschel, Felix Weber, Sebastian Pfaller

* Institute of Applied Mechanics
Friedrich-Alexander-Universität Erlangen-Nürnberg
Germany
e-mail: maximilian.ries@fau.de

Abstract:

Polymers are highly versatile materials whose mechanical performance can be further enhanced by adding nano-sized fillers. Due to their low density compared to conventional engineering materials, these polymer nanocomposites are often used as lightweight materials in the automotive and renewable energy industries. For the development of new polymer nanocomposites as well as for the design of structural components, accurate models are required, which take into account the polymers' molecular structure and the interaction with the nanofillers.

Such models are currently lacking, especially for the complex fracture behavior of polymer nanocomposites, which is significantly affected by molecular mechanisms. Hence, we propose a molecular dynamics model that represents a generic thermoplastic nanocomposite and features a physically sound bond-breaking criterion to facilitate the investigation of polymer fracture. To this end, molecular dynamics is well suited to resolve the molecular scale and analyze the effect of the nano-fillers on crack propagation. Furthermore, to be able to consider sufficiently large samples despite the high computational costs of molecular dynamics, we calibrate a coarse-grained model and present first results under periodic boundary conditions.

These studies are, of course, only a first step toward understanding polymer fracture. Moreover, our molecular models cannot be applied to engineering problems due to their long computation times. Thus, we plan to transfer our findings to more efficient continuum mechanical models using a multiscale approach. Such molecular-informed models would help exploit the full potential of polymer nanocomposites in their development and application.

Keywords: polymers, polymer nanocomposites, fracture, molecular dynamics, coarse graining

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Personalized adaptation of computational bone remodelling models from medical images

E. Nadal[1,*], J. Gutiérrez-Gil[1], C.M. Atienza[2], M. Tur[1], and J.J. Ródenas[1]

[1] Instituto de Ingeniería Mecánica y Biomecánica (I2MB)
Universitat Politècnica de València. Valencia, España.
e-mail: jorgugi1@upv.es, ennaso@upvnet.upv.es, {manuel.tur, jjrodena}@mcm.upv.es

[2] Instituto de Biomecánica de Valencia (IBV). Valencia, España.
e-mail: carlos.atienza@ibv.org

Keywords: Bone Remodelling, Image-Based Finite Element Analysis, Biological Factors, Personalized medicine

Abstract

In the literature related to the simulation of bone remodeling, it is usual to generically estimate the imposed structural boundary conditions and the biological parameters included in the formulation of the remodeling algorithms, introducing significant modeling errors. Since the actual measurement of modeling conditions in each patient is not accessible in a standard medical protocol, a procedure is proposed to adjust said conditions from the computed axial tomography (CT) image, normally performed for diagnosis.

In this work we try to find the patient specific reference stimulus, which in combination of the mechanical loads describes the bone evolution [1]. The reference stimulus is considered as a bibliography input [1] or adjusted for obtaining expected results [4] since the experimentation is difficult and only one publication is found in humans [5]. In order to circumvent this problem an approach based on the mechanostat theory [3] is proposed where depending on the load scenario a bone strain window is selected and the reference stimulus is numerically evaluated.

In this case, we apply the methodology to a femur where the loads are supposed to be known. For a given load scenario, the reference stimuli can be inferred according to the mechanostat theory, where the strains are evaluated by the cgFEM tool [2]. The mechanostat theory reveals that there exist a strain window where the bone remains comfortable, that is no overload, which would generate damage, and no underload, which would generate absorption. Different authors proposes some windows and the reference stimuli obtained is compared with experimental results performed over a human tibia [5]. The selection of the best window is guided by the minimization of the bone remodelling with the reference stimuli evaluated. Finally, the results are compared with the bibliography reference stimuli for long bone, achieving a better personalized adaptation when the proposed technique is used.

1 Acknowledgements

Thea authors thanks the support of Generalitat Valenciana (FEDEGENT/2018/025) y (Prometeo/2021/046 and CIAICO/2021/226), Ministerio de Economía, Industria y Competitividad (DPI2017-89816-R) y FEDER.

References

[1] Doblaré, M. and García, J.M. Anisotropic bone remodelling model based on a continuum damage-repair theory. *Journal of Biomechanics*, Vol. **35**, pp.1–7, (2002).

[2] Direct medical image-based Finite Element modelling for patient-specific simulation of future implants. *Finite Elements in Analysis and Design*, Vol. **136**, pp. 37–57, (2017).

[3] H. M. Frost Bone "Mass" and the "Mechanostat": A Proposal, The Anatomic Record, **219**, pp. 1-9, 1987.

[4] J. Gutiérrez-Gil, E. Nadal, K. Bouza, M. Tur, C.M. Atienza, O. Allix, J.J. Ródenas, Bone remodelling-based numerical evaluation of personalized masticatory forces from CT-scans, Computer Methods in Applied Mechanics and Engineering, **401**, 115635, 2022.

[5] L. E. Lanyon, W. G. J. Hampsona, E. Goodship, J. S. Shah, Bone Deformation Recorded In Vivo From Strain Gauges Attached To The Human Tibial Shaft, Acta Orthopaedica Scandinavica, **46**, pp. 256-268, 1975.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Image-derived biomechanical properties of aortic walls in Marfan syndrome

Rosnel Claire*, Capelli Claudio†, Schievano Silvia†, Sivera Raphael† and Aggarwal Ankush*

* Computational Biomechanics Research Group
Glasgow Computational Engineering Centre (GCEC), University of Glasgow
Glasgow, United Kingdom
e-mail: claire.rosnel@glasgow.ac.uk

† Institute of Cardiovascular Science
University College London
London, United Kingdom
e-mail: r.sivera@ucl.ac.uk

Abstract: In patients with Marfan Syndrome (MFS), aortic walls present altered elastic behaviour and an increased stiffness that lead to aortic dilatation in 50% to 60% of adults patients (Ammash et al., 2008). A common treatment to avoid fatal rupture of the dilated aortas is prophylactic surgery. Despite the aortic diameter being a guideline for prophylactic surgery, studies have shown that biomechanical properties change at early stages of the disease and often before any changes in the aortic diameter. In this study, we present a framework that combines advanced in-vivo imaging and computational modelling to estimate biomechanical properties of MFS tissues and compare them to healthy patients. Direct measurements on the echocardiograms and magnetic resonance images (MRIs) were used to calculate patient-specific aortic stiffness measurements. A statistical analysis showed a significant difference in aortic stiffness between Marfan and control. A classical fitting method and a Bayesian approach were also used to determine a hyperelastic law that best describes Marfan aortic walls' behaviour. This model selection technique demonstrated that for connective tissue disorders such as MFS, fitted hyperlelastic model and corresponding parameters differ from control. Our results demonstrate that computational modelling can be a promising tool to understand aortic behaviour for Marfan patients and predict dilatation at an early stage.

Keywords: Marfan Syndrome, Aorta, In-vivo imaging, Biomechanics, Stiffness, Model selection

1 Introduction

Marfan syndrome (MFS) is an inherited genetic condition affecting connective tissues and exposing patients to life-threatening cardiovascular complications. This condition causes elastin degradation and leads to stiffening and dilatation of aortic walls, thus increasing the risk of aneurysms and dissection. The current clinical guideline is measuring the aorta's diameter to assess the need of prophylactic surgery [1]. However, studies have demonstrated that changes in the biomechanical behaviour could be an early marker of aortic disease [2][3]. Knowing detailed biomechanical properties of aortic walls and being able to model them accurately is thus truly important to diagnose MFS at an early stage, explain how aneurysms grow and point to strategies to prevent them. The aim of this study is to present a framework that combines advanced in-vivo imaging and computational modelling to directly estimate biomechanical properties of MFS tissues in-vivo and compare them to healthy patients as controls.

2 Materials and methods

A combination of cardiovascular imaging modalities served as a dataset: Echocardiograms and MRIs of Marfan and healthy patients were used to extract the time evolution of the geometry over a cardiac cycle, or over different time points in the patient's life. Segmentation and processing methods were used to derive strain, deformation measures and other indexes of aortic stiffness such as distensibility, defined as the relative change in volume per unit of pressure, and beta stiffness index, defined as log of the pressure ratio divided by the relative change in diameter. A statistical analysis was performed to compare MFS and control, and correlation tests investigated which parameter is the best predictor of aortic dilatation. Finally, a classical fitting method and Bayesian approach were compared to find a constitutive model that best describes Marfan aortic tissues.

3 Results

Cross-sectional views of the aorta allowed to measure the aortic diameter during the cardiac cycle. Preliminary results demonstrated that Marfan patients show different elastic properties compared to control. A classical fitting method and a Bayesian approach were tested on control data and identified a hyperelastic constitutive model and corresponding parameters that best describe the aortic root walls' behaviour. The same model selection method is to be applied on Marfan data.

4 Conclusions

Computational techniques using in-vivo images to directly extract deformation measures show promising results in understanding biomechanical properties in Marfan patients. In this study, we have shown that diameter alone is not the best predictor of aortic disease. Early results showed an impaired elastic behaviour of Marfan tissue at an early stage. Computational modelling allowed us to identify a constitutive model to describe the altered biomechanical behaviour.

References

[1] Shiv Kumar Choudhary and Aayush Goyal. Aortic root surgery in Marfan syndrome. *Indian Journal of Thoracic and Cardiovascular Surgery : Official Organ, Association of Thoracic and Cardiovascular Surgeons of India*, 35(Suppl 2):79–86, June 2019.

[2] Gisele Teixido-Tura, Alban Redheuil, Jose Rodriguez-Palomares, Laura Gutierrez, Violeta Sanchez, Alberto Forteza, Joan A.C. Lima, David Garcia-Dorado, and Artur Evangelista. Aortic biomechanics by magnetic resonance: Early markers of aortic disease in Marfan syndrome regardless of aortic dilatation? 2014.

[3] Parmanand Singh, Zaid Almarzooq, Noel C. F. Codell, Yi Wang, Mary J. Roman, Richard B. Devereux, and Jonathan W. Weinsaft. Cine-CMR partial voxel segmentation demonstrates increased aortic stiffness among patients with Marfan syndrome. *Journal of Thoracic Disease*, 9(Suppl 4):S239–S245, April 2017.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Global sensitivity analysis of complex biomechanical models

Sebastian Brandstaeter*, Barbara Wirthl†, Jonas Nitzler† and Wolfgang A. Wall†

* Institute for Mathematics and Computer-Based Simulation
University of the Bundeswehr Munich
Neubiberg, Germany
e-mail: sebastian.brandstaeter@unibw.de

† Institute for Computational Mechanics
Technical University of Munich
Garching, Germany
e-mail: barbara.wirthl@tum.de, jonas.nitzler@tum.de, wolfgang.a.wall@tum.de

Abstract: Biomechanical models often contain many parameters. Global sensitivity analysis can identify the most influential and the non-influential parameters. This allows, for example, to focus identification efforts on the influential parameters. Here, we show how to apply variance-based global sensitivity analysis to complex biomechanical models using Gaussian-process surrogate models. We exemplify the approach for a tumour-growth model and a model of aneurysm formation. We find that often a few influential parameters dominate the model output variance. Furthermore, there can be significant amounts of parameter interactions highlighting the need for global methods. In summary, Gaussian-process based global sensitivity analysis is both feasible and valuable for complex, computationally expensive biomechanical models and particularly for their reliable predictive use in the clinical practice.

Keywords: global sensitvity analysis, Sobol's method, biomechanics, aneurysm formation, tumour growth

1 Introduction

Biomechanical models often contain a myriad of parameters. Lack of knowledge on these parameters naturally results in uncertainty that should be accounted for. Parameter identification can help reduce this uncertainty. However, the identification of all parameters is not feasible. Therefore, variance-based global sensitivity analysis is a task of great importance. While naturally considering the uncertainty, it enables the separation of the influential from the non-influential parameters. This allows to use resources efficiently, for example, by focusing patient-specific identification efforts on the most influential parameters and justifying the use of population average values for the non-influential parameters.

2 Methodology and results

In this contribution, we show how to apply Sobol's variance-based global sensitivity analysis to complex biomechanical models by making use of Gaussian-process surrogate models. We follow the approach of Le Gratiet et al. [1], which not only allows for the quantification of the total uncertainty in the estimates of the sensitivity indices but also of the individual contributions arising from surrogate model and Monte-Carlo integration, respectively.
By applying the approach to multiple sophisticated examples including nanoparticle-mediated drug delivery in a multiphase tumour-growth model [2] and aneurysms in a model of aortic

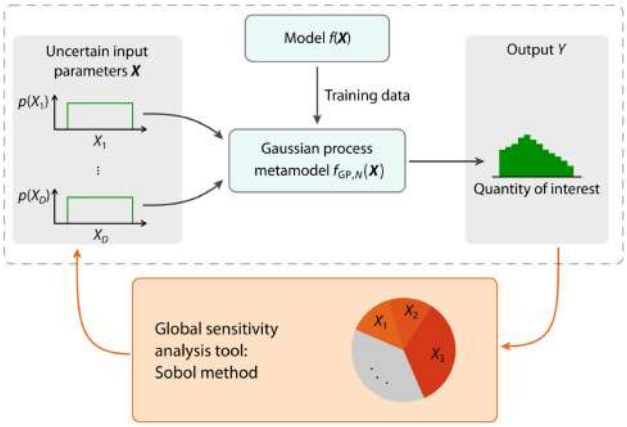


Figure 1: Overview of Sobol's variance-based global sensitivity based on Gaussian-process surrogate models. Reprinted from [2], licensed under a Creative Commons Attribution 4.0 International License (CC BY 4.0).

growth and remodelling [3], we demonstrate its benefit for biomechanical models.
From a methodological perspective, we find that separating influential and non-influential parameters requires a relatively small number of full model evaluations. However, computing accurate values for the sensitivity indices requires additional evaluations. In return, the extra effort enables the estimation of higher-order indices.
From a biomechanical modelling perspective, we find that the model output variance is often dominated by a few influential parameters. Furthermore, there can be significant amounts of parameter interactions, which highlights the need for global rather than local sensitivity analysis when studying the parameter sensitivities of complex biomechanical models.

3 Conclusion

In summary, our results demonstrate that Gaussian-process based global sensitivity analysis is both feasible and valuable for complex, computationally expensive biomechanical models. It can be particularly useful as a part of parameter identification and model oder reduction. In the big picture of reliable predictive model use in the clinical practice, we believe that the presented workflow should become an essential part of the model development process.

References

[1] Le Gratiet L, Cannamela C, Iooss B. A Bayesian Approach for Global Sensitivity Analysis of (Multifidelity) Computer Codes. J Uncertain Quantif 2014;2:336–363. DOI: 10.1137/130926869.

[2] Wirthl B, Brandstaeter S, Nitzler J, Schrefler, BA, Wall WA. Global sensitivity analysis based on Gaussian-process metamodelling for complex biomechanical problems. Int J Numer Meth Biomed Engng 2023;e3675. DOI: 10.1002/cnm.3675.

[3] Brandstaeter S, Fuchs SL, Biehler J, Aydin, RC, Wall WA, Cyron CJ. Global Sensitivity Analysis of a Homogenized Constrained Mixture Model of Arterial Growth and Remodeling. J Elast 2021;145:191–221. DOI: 10.1007/s10659-021-09833-9.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A general Bayesian framework for calibrating constitutive models

Wollner, M.P.[1], **Terzano, M.**[1], **Rolf-Pissarczyk, M.**[1] **and Holzapfel, G.A.**[1,2]

[1] Institute of Biomechanics
Graz University of Technology
Graz, Austria
e-mail: wollner@tugraz.at

[2] Department of Structural Engineering
Norwegian University of Science and Technology (NTNU)
Trondheim, Norway
e-mail: holzapfel@tugraz.at

Abstract: As the demand for verification of simulations increases, the propagation of uncertainties from experiment to model has become a necessity (ASME, 2019; FDA, 2021). The calibration of material constants by minimizing some cost function, e.g., least squares, is widely adopted, but does not provide probabilistic insights (Destrade, 2017). In addition, the weighting of different types of experimental setups leaves considerable ambiguity. To overcome these drawbacks, we construct a probability distribution with respect to the parameters of any constitutive model for any number of experiments. We employ a Bayesian framework with a Gaussian-based likelihood and Jeffrey's prior (Ranftl, 2022). After marginalizing out unknown experimental variances, a parametrization-invariant posterior remains, similar to Student's t-distribution. Statements can now be made about the probability that sets of material constants reflect the experimental data on average. Since the resulting posterior is a proper probability density, all relevant probabilistic operations can be performed on it, such as the identification of modes or the sampling of parameter sets, which in turn can be used to propagate the experimental uncertainty to subsequent simulations independently of the calibration data. We demonstrate the approach for an anisotropic material model using different types of mechanical experiments.

Keywords: Uncertainty Propagation, Bayesian Calibration, Constitutive Modeling

References

ASME V&V Committee. Standard for Verification and Validation in Computational Solid Mechanics. ASME, New York, USA; 2019.

FDA Center for Devices and Radiological Health. Assessing the Credibility of Computational Modeling and Simulation in Medical Device Submissions. FDA, Rockville, USA; 2021.

Destrade M, Saccomandi G, Sgura I. Methodical fitting for mathematical models of rubber-like materials. Proc R Soc A 2017;473:20160811.

Ranftl S, Müller TS, Winderberger U, Brenn G, von der Linden W. A Bayesian approach to blood rheological uncertainties in aortic hemodynamics. Int J Numer Meth Biomed Engng 2022;e3576.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Development of representative artery models for stent fatigue tests

Jude Mohamed Osman Hussain*, **Ankush Aggarwal*** **and Andrew McBride***

* University of Glasgow
Glasgow, United Kingdom
j.mohamed-osman-hussain.1@research.gla.ac.uk

Abstract: Fatigue conditions of endovascular stents are difficult to predict computationally given their dependence on the arterial representation. Aleatory and epistemic uncertainty arise from the uncertainty in the deduction of material parameter values and the choice of constitutive models, respectively. To account for such uncertainties, a systematic approach to selecting hyperelastic models that outlines objective criteria for a parsimonious model in capturing arterial compliance is necessary. A Bayesian approach to hyperelastic model selection and parameter identification for arterial wall modeling is thus detailed and proposed. This framework employs pre- and postoperative compliance data of abdominal aortic aneurysms (AAA) patients treated with the self-expanding stent-graft, the *Anaconda*^{TM}, to inform the choice of a representative hyperelastic model for computational fatigue testing.

Keywords: Bayesian model selection, parameter identification, uncertainty quantification

1 Introduction

To better understand failure stent fatigue conditions in-vivo, a simplified kinematic model of the stent-artery system [1] through which model and parameter probabilities are updated with patient compliance data aids the calibration of model and parameter choices.

1.1 Patient sample, arterial kinematics, and Bayesian model selection

Anonymized collected data $\mathbf{d}_{\text{pat}}$ of the AA[1] of 15 patients who underwent EVAR[2] treatment with the *Anaconda*$^{\text{TM}}$ stent-graft include preoperative measures, $\text{v}_{\text{pre}} = \begin{bmatrix} r_{\text{dias,pre}} & \text{p}_\Delta \end{bmatrix}$, i.e. diastolic radius $\text{r}_{\text{dias,pre}}$ and pulse pressure p_Δ. Postoperative measures $\text{v}_{\text{post}} = \begin{bmatrix} d_{\text{post}} & \varepsilon \end{bmatrix}$ include the compliance d_{post} and expansion ε[3]. Preoperative compliance d_{pre} was not measured for patients and is obtained from literature as $\mathbf{d}_{\text{lit}}$.

$$d_{\text{post}} = \frac{\text{r}_{\text{sys,post}} - \text{r}_{\text{dias,post}}}{\text{r}_{\text{dias,post}}\ \text{p}_\Delta}, \quad \varepsilon = \frac{\text{r}_{\text{dias,post}} - \text{r}_{\text{dias,pre}}}{\text{r}_{\text{dias,pre}}}, \quad d_{\text{pre}} = \frac{\text{r}_{\text{sys,pre}} - \text{r}_{\text{dias,pre}}}{\text{r}_{\text{dias,pre}}}. \tag{1}$$

The AA is modeled as an incompressible hyperelastic tube subject to axisymmetric deformation. The tube begins at stress-free configuration Ω_0, where R_i is the inner radius in the reference configuration. After loading by a chronic outward force f_0 and blood pressure p_Δ, the inner radius r_i and p_Δ in the loaded configuration Ω_{L} are [1]

$$\Omega_0 \mapsto \Omega_{\text{L}} : r(R) = \sqrt{\frac{R^2 - R_i^2}{\lambda_z} + r_i^2}, \quad \text{p}_\Delta = \int_{r_i}^{r_o} \left(\lambda_\theta \frac{\partial \Psi}{\partial \lambda_\theta} - \lambda_r \frac{\partial \Psi}{\partial \lambda_r} \right) \frac{\text{d}r}{r}. \tag{2}$$

[1] abdominal aorta
[2] Endovascular aneurysm repair
[3] In Eq. 1, subscripts $_{\text{post,dias}}$, and $_{\text{sys}}$ denote the postoperative, diastolic, and systolic states, respectively.

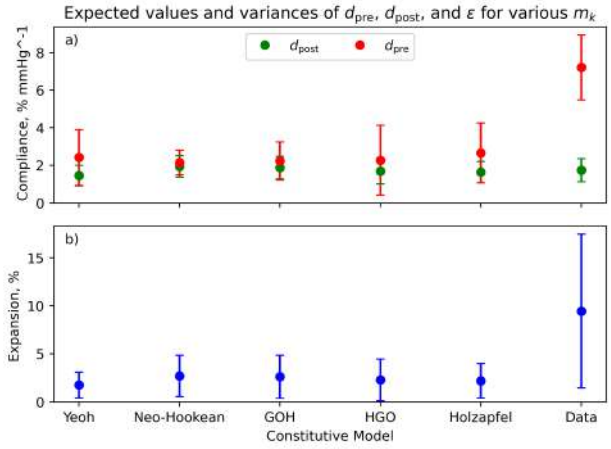


Figure 1: Expected values of d_{pre} and d_{post}, and (b) ε compared to $\mathbf{d}_{\text{pat}}$ and $\mathbf{d}_{\text{lit}}$ ("Data").

Table 1: Normalized evidence and maximum likelihood estimates of θ_k for three models with greatest evidence values.

	NH	GOH	Holzapfel
Evidence	1.00	0.61	0.35
θ_1 (kPa)	$\mu = 30.3$	$k_1 = 14.1$	$k_1 = 47.4$
θ_2	–	$k_2 = 29.0$	$k_2 = 13.5$
θ_3	–	$\kappa = 0.11$	$\kappa = 0.98$
θ_4 (kPa)	–	$\mu = 98.4$	$\mu = 98.1$

where λ_r, λ_θ, and λ_z are the principal stretches in cylindrical coordinates, r_{o} is the outer radius, and Ψ is the hyperelastic strain energy density. The *Anaconda*$^{\text{TM}}$ is modeled as a locally linear spring with force $F = k\,(r_{\text{dias,post}} - r_{\text{dias,pre}}) + f_0$, where k is the stent stiffness. Bayes' theorem is used to update uniform prior distributions $p\,(\theta_k|\text{m}_k)$ of parameters θ_k with patient data $\mathbf{d}$ using constitutive model m_k resulting in the posterior distribution $p\,(\theta_k|\mathbf{d}, \text{m}_k)$

$$p\,(\theta_k|\mathbf{d}, \text{m}_k) = \frac{p\,(\mathbf{d}|\theta_k, \text{m}_k)\,p\,(\theta_k|\text{m}_k)}{p\,(\mathbf{d} \mid \text{m}_k)}. \tag{3}$$

$p\,(\mathbf{d}|\theta_k, \text{m}_k)$ is the likelihood of observing patient data $\mathbf{d}_{\text{pat}}$ and $\mathbf{d}_{\text{lit}}$ given m_k and corresponding θ_k. Candidate models m_k include the Yeoh, Neo-Hookean (NH), GOH, Holzapfel, and HGO models [2]. The evidence $p\,(\mathbf{d} \mid \text{m}_k) = \int_{\boldsymbol{\theta}_k} p\,(\mathbf{d}|\theta_k, \text{m}_k)\,p\,(\theta_k|\text{m}_k)$ is approximated using Monte Carlo integration. d_{post}, ε, and d_{pre} are calculated using Eq.2 and 1, and their expected values $\mathbb{E}$ are calculated as $\mathbb{E}\,(\text{v}_{\text{post}}) = \int_{\theta_k} \text{v}_{\text{post}}\,(\theta)\,p\,(\theta \mid \mathbf{d})\,\text{d}\theta$.

2 Conclusions

Fig. 1 compares the expected values of d_{pre}, d_{post}, and ε from various m_k to $\mathbf{d}_{\text{pat}}$ and $\mathbf{d}_{\text{lit}}$, and Table 1 outlines evidence values and maximum likelihood estimates (MLEs) for models with the highest evidences. Given that all models similarly capture $\mathbf{d}_{\text{pat}}$ and $\mathbf{d}_{\text{lit}}$ in Fig. 1, the NH model has the highest evidence given its 2-termed nature. The outlined framework shows great promise in assisting the development of representative artery models.

3 Acknowledgements

J.H. acknowledges funding from the Engineering and Physical Sciences Research Council.

References

[1] Auricchio, F. et al. (2014) How constitutive model complexity can affect the capability to fit experimental data: A focus on human carotid arteries and extension/inflation data. Archives of Computational Methods in Engineering, 21(3), pp. 273–292.

[2] Aggarwal, A. et al. (2023) A bayesian constitutive model selection framework for biaxialmechanical testing of planar soft tissues: Application to porcine aortic valves. Journal of the Mechanical Behavior of Biomedical Materials, 138, p. 105657.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Analysis of Lueders bands and Portevin Le-Chatelier effect using experimental and computational data

Mucha Marzena[*†], Rose Lars[*], Wcisło Balbina[†], Menzel Andreas[*‡] and Pamin Jerzy[†]

[*] Institute of Mechanics
Department of Mechanical Engineering, TU Dortmund University
Dortmund, Germany
e-mail: Marzena.Mucha@tu-dortmund.de

[†] Chair for Computational Engineering
Department of Civil Engineering, Cracow University of Technology
Cracow, Poland

[‡] Division of Solid Mechanics
Department of Construction Sciences, Lund University
Lund, Sweden

Abstract: This work is focused on the analysis of Lueders bands and Portevin Le-Chatelier (PLC) effect using experimental and computational data. The Lueders bands are related to the initiation of localization bands and movement of fronts of the underlying plastic zones. The PLC effect is associated with Dynamic Strain Aging and caused by interactions between solute atoms and mobile dislocations during plastic processes. Tensile tests of aluminum alloy AW5083 specimens have been conducted for three strain rates at room temperature. Both Lueders and PLC bands are reflected by the obtained force-displacement diagrams. Displacement and temperature fields are recorded during the experiments. A large strain thermo-viscoplasticity model with the Estrin-McCormick model, enhanced by switch functions, is applied in simulations, whereby good agreement between experimental data and computed results is obtained.

Keywords: Lueders bands, PLC effect, large strains, thermo-viscoplasticity, Estrin-McCormick model

1 Introduction

Both Lueders bands and Portevin Le-Chatelier (PLC) effect can be observed in certain aluminum alloys and steels, depending on strain rate and temperature. They can appear in a sequence along a loading path, see [1]. Lueders bands can be observed when the fronts of plastic zones related to first localization bands move through the specimen. The PLC effect is commonly associated with Dynamic Strain Aging and negative strain rate sensitivity. On the macroscopic level serrations, which are repetitive changes from softening to hardening, occur in the force-displacement diagram and corresponding shear bands can be observed in the sample. On the microscopic level such effects are caused by interactions of solute atoms with mobile dislocations during plastic deformation, see [2].

2 Experimental and computational results

Experiments are performed in tensile machine using bone-shape samples made of aluminium alloy AW5083 at room temperature for three strain rates ($\dot{\varepsilon} = \{10^{-4}, 10^{-3}, 10^{-2}\}\ \mathrm{s}^{-1}$). A DIC

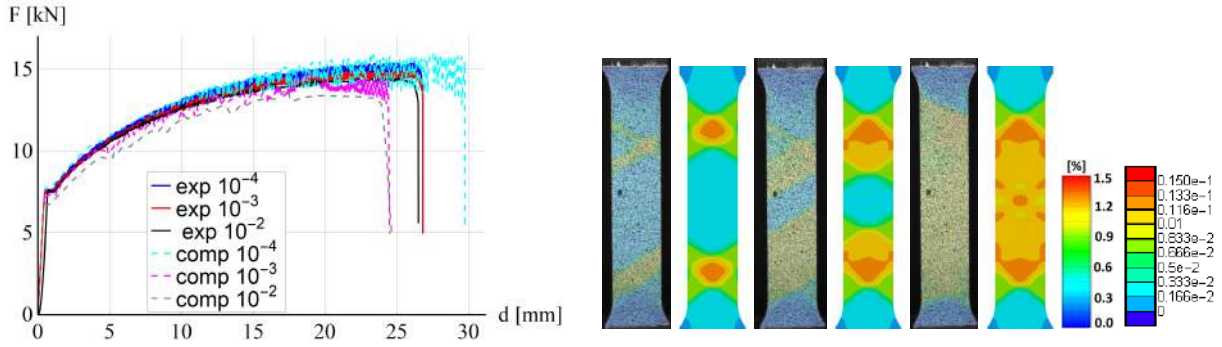


Figure 1: Total reaction force vs. sample elongation (left) and distribution of longitudinal engineering strain for experiments and simulations during Lueders band propagation process at selected time steps (right).

system and a thermal camera are used to monitor full field data during the loading processes. Simulations are performed using a large-strain thermo-visco-plasticty model, which is based on [3]. Lueders bands are modelled with multi-linear hardening contributions and the PLC effect is captured by the Estrin-McCormick model, see [4], with switching functions to combine the two model components. Fig. 1 (left) shows the total reaction force vs. sample elongation for different strain rates, which illustrates the Lueders bands phase followed by saturation hardening with PLC serrations and final failure. Computational predictions (comp) qualitatively match experimentally measured data (exp). Fig. 1 (right) presents the distributions of longitudinal engineering strain for selected time steps in the initial phase of loading. Two bands are formed then in the top part and in the bottom part of the sample. They move through the sample towards its center and eventually merge.

3 Conclusions

A good agreement between experimental data and computational predictions is achieved, in particular when load–displacement diagrams for different loading rates are concerned.

4 Acknowledgements

The work is supported by National Science Centre of Poland (grant 2018/31/N/ST8/03573).

References

[1] Bergstrom Y, Roberts W. The application of dislocation model to dynamic strain ageing in α-iron containing interstitial atoms. Acta Metallurgica 1971; 19:815-823.

[2] Cottrell AH, Bilby BA. Dislocation theory of yielding and strain ageing of iron. Proc. Phy. Soc. Sect. A. 1949; 62(1):49-62.

[3] Mucha M, Wcisło B, Pamin J. Simulation of Lueders bands using regularized large strain elasto-plasticity. Arch. Mech. 2021; 73(1):83–117.

[4] Böhlke T, Bondár G, Estrin Y, Lebyodkin MA. Geometrically non-linear modeling of the Portevin-–Le Chatelier effect. Comput. Mat. Sci. 2009; 44(4):1076-1088.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Homogenization of phase-field evolution laws based on unequally and nonlinearly weighted averaging operators

Vincent von Oertzen*, **Bjoern Kiefer***

* Institute of Mechanics and Fluid Dynamics (IMFD)
Applied Mechanics – Solid Mechanics, TU Bergakademie Freiberg
Lampadiusstr. 4, 09599 Freiberg, Germany
e-mail: vincent.von-oertzen@imfd.tu-freiberg.de

Abstract: The phase-field approach has manifested itself as an efficient and widely applicable method to describe the behavior of continua in which the evolution of complex interface topologies is a dominant physical mechanism. Even though many important contributions were made over the last decade in corresponding areas of fracture mechanics and multi-physics problems, a general concept for consistently transferring transient phase-field model information between several spatial, and also temporal, scales has still not been fully developed. More specifically, current homogenization frameworks typically rely on many additional assumptions strongly restricting the space of microscopic field distributions. To address this issue, the notion of unequally and nonlinearly weighted averaging operators was recently introduced in [1]. Here, this general approach is applied to dual-phase systems in order to determine effective driving forces and thus also derive the corresponding spatially and temporally homogenized evolution laws by simultaneously reducing the number of assumptions that need to be made on the microscale.

Keywords: Phase-field Modeling, Homogenization, Scale-Bridging

1 Introduction

Within every phase-field approach, mixture rules have to be formulated in order to describe the interpolation between single-phase properties inside diffuse interface regions. As a consequence, there exist a variety of well-established interpolation schemes, see [2] and the references therein, resulting in deviating driving forces contributions and thus leading to different microstructure predictions under multiple loading scenarios. Despite the fact that assumptions on the microscopic phase morphology may differ between each approach, based on the underlying physical transformation mechanisms, most of these models have in common that assumptions were made on field variables that are microscopically related in rate-independent form, whereas their macroscopic counterparts are usually associated with transient problems, see [1, 2]. Clearly, the question arises, how respective time derivatives can be involved within evolution equations on the next larger spatial scale if they do not appear on the underlying microscopic scale. To overcome this problem, the concept of unequally and nonlinearly weighted averaging operators is applied to a dual-phase system in order to derive spatially and temporally homogenized evolution laws as the result of an already transient evolution framework formulated on the microscopic scale.

2 Mathematical considerations and homogenization procedure

Consider an Allen-Cahn type evolution law of the general form $\dot{\eta} = f(\eta, \boldsymbol{\nabla} \otimes \boldsymbol{\nabla}\eta, \theta)$ relating phase morphologies $\eta(\boldsymbol{X}, t)$ with fluctuating temperature fields $\theta(\boldsymbol{X}, t)$ $(\forall \boldsymbol{X} \in \mathcal{B}$ and $\forall \boldsymbol{t} \in \mathcal{T})$. Furthermore, let $\mathcal{Q} := \{\eta, \dot{\eta}, \boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\eta, \theta\}$ denote the set of microscopic field quantities and ${}_{\kappa}\mathcal{W}_{\boldsymbol{\alpha}}$ the set of nonlinear, spatial weighting functions ${}_{\kappa}\boldsymbol{\Phi}_{\boldsymbol{\alpha}} : \mathcal{Q} \times \mathcal{B} \times \mathcal{T} \to \mathbb{R}^{\dim(\boldsymbol{\alpha})}$ defined for each $\boldsymbol{\alpha} \in \mathcal{Q}$. In what follows, the abbreviation ${}_{\kappa}\boldsymbol{\Phi}_{\boldsymbol{\alpha}}(\boldsymbol{\beta}(\boldsymbol{X}, t), \boldsymbol{X}) := {}_{\kappa}\boldsymbol{\Phi}^{\boldsymbol{\beta}}_{\boldsymbol{\alpha}}$ is used according to [1]. Based on the spatial averaging operator $\langle \square \rangle_{\mathcal{B}} := \frac{1}{V(\mathcal{B})} \int_{\mathcal{B}} \square \, \mathrm{d}V$, the developed homogenization procedure aims to find finitely many weighting functions ${}_{\kappa}\Phi_{\eta,i} \in {}_{\kappa}\mathcal{W}_{\eta}$ $(i = 0, ..., N$ with ${}_{\kappa}\Phi_{\eta,0} := \eta)$, combined with functional relations $\mathcal{F}_i$, generating a system of ordinary differential equations of the type:

$$\langle {}_{\kappa}\dot{\Phi}^{\eta}_{\eta,i} \rangle_{\mathcal{B}} = \langle \partial_{\eta} \, {}_{\kappa}\Phi^{\eta}_{\eta,i} \, f(\eta, \boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\eta, \theta) \rangle_{\mathcal{B}} = \mathcal{F}_i \oint \langle \eta \rangle_{\mathcal{B}}, \langle {}_{\kappa}\Phi^{\eta}_{\eta,1} \rangle_{\mathcal{B}}, ..., \langle {}_{\kappa}\Phi^{\eta}_{\eta,N} \rangle_{\mathcal{B}}, \langle \theta \rangle_{\mathcal{B}} \big) \ . \tag{1}$$

Solutions of this system give rise to a macroscopic description of phase evolution incorporating generalized degrees of freedom $\langle {}_{\kappa}\Phi^{\eta}_{\eta,i} \rangle_{\mathcal{B}}$ that characterize the effective phase morphology.

3 Conclusions

It is found that choosing appropriate weighting functions decreases the span of effective driving forces, see Figure 1, by simultaneously reducing the number of necessary assumptions which need to be made on microscopic order distributions. Furthermore, numerical solutions of (1) are shown to match—up to a negligible tolerance—those obtained from Allen-Cahn based finite element simulations of microstructure evolution in ZrO_2 for various temperature-induced loading scenarios thus validating the outlined homogenization procedure.

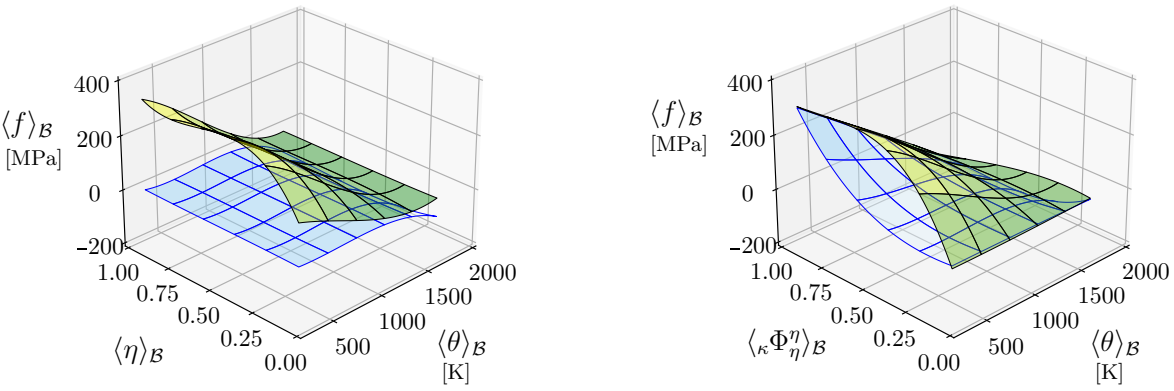


Figure 1: Bounds of effective driving forces in ZrO_2 based on conventionally averaged phase states $\langle \eta \rangle_{\mathcal{B}}$ (left) and nonlinearly weighted averages $\langle {}_{\kappa}\Phi^{\eta}_{\eta} \rangle_{\mathcal{B}}$ (right), evaluated for various phase morphologies.

References

[1] Von Oertzen V, Kiefer B. Unequally and non-linearly weighted averaging operators as a general homogenization approach for phase-field modeling of phase transforming materials. Shape Mem Superelasticity 2022;8:425–437.

[2] Kiefer B, Furlan T, Mosler J. A numerical convergence study regarding homogenization assumptions in phase field modeling. Int J Numer Methods Eng 2017;112(9):1097–1128.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A coupled phase-field and crystal-plasticity model for twinning and plastic slip

Mohsen Rezaee-Hajidehi[†], Przemysław Sadowski[†] Stanisław Stupkiewicz[†]

Institute of Fundamental Technological Research (IPPT), Polish Academy of Sciences
Warsaw, Poland
e-mails: mrezaee@ippt.pan.pl, psad@ippt.pan.pl, sstupkie@ippt.pan.pl

Abstract: Deformation twinning is a prevalent inelastic deformation mechanism in certain metals and alloys. Modeling twinning poses additional challenges in comparison to plastic slip due to the critical differences in the underlying mechanism and characterisitcs. In this study, we develop a finite-element-based model for coupled twinning and plastic slip by combining the phase-field method and crystal plasticity. A key feature of our model is the treatment of twinning as a displacive transformation, as in martensitic phase transformation, where the twinning kinematics is characterized by a volume-preserving stretch followed by a rigid-body rotation, in contrast to the conventional approach based on a simple shear. This approach is particularly relevant when conjugate twinning systems are crystallographically equivalent. In the diffuse-interface phase-field framework, it enables to use a single order parameter to describe the two conjugate twinning systems. To demonstrate the capabilities of our model, we develop a computational model for magnesium with an HCP crystal structure and study various problems including twin nucleation, twin evolution and transmission through grain boundaries, and its interaction with plastic slip.

Keywords: Deformation twinning, Microstructure, Phase-field method, Crystal plasticity, Finite-element framework

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A phase-field model for ferroelectrics with nonlinear kinetics and electro-mechanical couplings

Laurent Guin*, Hsu-Cheng Cheng† and Dennis M. Kochmann†

* Department of Mechanics, Laboratory of Solid Mechanics
Ecole polytechnique
Palaiseau, France
e-mail: laurent.guin@polytechnique.edu

† Department of Mechanical and Process Engineering, Mechanics & Materials Lab
ETH Zurich
Zurich, Switzerland

Abstract: Phase field modeling has been widely applied to model the evolution of domain patterns in various phase transformation problems. Existing phase-field models for the evolution of domain structures in ferroelectrics are based on an Allen-Cahn-type evolution law. However, this evolution law, which assumes a linear kinetic relation between the thermodynamic driving force acting on a domain wall and the domain wall velocity, fails to capture rate effects in ferroelectrics. To overcome this limitation, we propose a new phase field model for ferroelectrics [1], one that incorporates nonlinearities in the kinetics of domain walls and fully accounts for electro-mechanical coupling. As a multi-phase-field generalization of the model of Alber & Zhu [2], it is based on the domain volume fraction of each variant as the primary phase field and incorporates the anisotropic dielectric, elastic, and piezoelectric properties of the different variants. With the ability to easily modify these different material properties, we investigate the relative contributions of electrostatics, mechanics, and piezoelectric effects to the motion of domain walls. The phase field model is validated through a comparison with the target sharp-interface model embedding nonlinear kinetics. Finally, limitations regarding the need to incorporate a separate nucleation process and open challenges (in common with all ferroelectric phase field models) with respect to the magnitude of the interfacial energy of domain walls are discussed.

Keywords: Ferroelectrics, phase-field model, phase transformation

References

[1] L. Guin, D. M. Kochmann, 2023, *A phase-field model for ferroelectrics with general kinetics. Part I: Model formulation.* arXiv preprint arXiv:2203.16479.

[2] H.-D. Alber, P. Zhu, 2013, *Comparison of a rapidely converging phase field model for interfaces in solids with the Allen-Cahn model.* Journal of Elasticity 111(2), 153–221.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A non-isothermal phase-field model based on the grand entropy

Ross Williams*, Simon Bray†, and Andrew McBride*

* Glasgow Computational Engineering Centre (GCEC)
James Watt School of Engineering, University of Glasgow
Glasgow, United Kingdom
e-mail: r.williams.2@research.gla.ac.uk

† Rolls-Royce plc
Derby, United Kingdom

Abstract: A phase-field model accounting for an arbitrary number of grains, phases, and chemical species is derived in a non-isothermal setting. Through the choice of the grand entropy (the Legendre transformation of the entropy functional) to govern the evolution of the system, physically-reasonable results, such as the conservation of mass, are guaranteed by the formulation. Details regarding current limitations and requirements of the formulation, as well as the calibration to data in order to represent realistic microstructures, is presented. The model based on the grand entropy, and solved using the finite element method, is benchmarked against isothermal and non-isothermal Fickian diffusion, and an established phase-field method for modelling multiple phases under isothermal conditions. The developed model is then used to study the evolution of a three-grain aggregate across a wide range of heating rates. Finally, the 2D microstructure of a nickel-based superalloy subjected to rapid heating via a Gleeble thermal-mechanical simulator and the friction welding process is investigated.

Keywords: Non-isothermal, Phase-field, Microstructure, Thermodynamics

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Constitutive model selection for sheet metal forming based on the analysis of identifiability of the material parameters

Mariana Conde[+,*], Sam Coppieters[†] and António Andrade-Campos[+]

[+] Department of Mechanical Engineering, TEMA - Centre for Mechanical Technology and Automation, LASI Associate Laboratory, University of Aveiro
Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

[†] Department of Materials Engineering, KU Leuven - Ghent Campus
Gebroeders De Smetstraat 1, Ghent, 9000, Belgium

[*]e-mail: marianaconde@ua.pt

Abstract: The efficient development and production of high-quality metal parts usually require realistic numerical simulations before the manufacturing procedure. The selection of the constitutive model has a considerable influence on the predicted material's behaviour and, consequently, on the simulation of the production process. A large number of constitutive models have been proposed to describe different mechanical phenomena. However, its selection is a laboured task that requires expertise. An inadequate choice of models can lead to errors in the numerical predictions and, thus, large costs and delays in the manufacturing procedure. An automatic constitutive model selection tool, as a recommendation engine, is the answer to solve this issue. This work aims to compare the quality of the models for a simulation of a DP600 steel. The approach is based on the identifiability analysis that considers the strain gradient variation due to the perturbation of the constitutive parameters. With this approach, it is possible to investigate if a constitutive model is adequate for calibration and reproduction of the material behaviour at hand.

Keywords: Constitutive model selection, Sheet metal forming, Finite Element Analysis, Identifiability

1 Introduction and literature review

The automotive and aircraft industries usually require high quality in their products and short time-to-market. Their efficiency relies, among others, on the correctness of the Finite Element Analysis (FEA) of the forming processes. However, in some cases, the lack of knowledge and time to correctly describe the material's behaviour is observed. This can lead to errors in the numerical simulations and, consequently, large costs and delays. To have material behaviour predictions, it is necessary to select an adequate constitutive model and correctly identify the corresponding material parameters. In the last decades, a large number of models were developed, implemented in numerical simulations and validated experimentally [1, 2]. The choice of the constitutive models that describe the material behaviour is an issue that a Finite Element Analysis (FEA) software user faces. Its selection for a specific material and process requires high expertise, an exhaustive investigation and mechanical experimentation. Many authors have been comparing simulations with different models with experimental data and finding which is more adequate for a specific material and process mainly based on trial-and-error approaches [1, 3, 4, 5]. Yet, this comparison can be very time-consuming, requiring several mechanical experiments, the calibration of the different

models, the simulation of a process and its validation. Thus, a flexible and automatic tool or strategy for model selection is lacking in the industry and scientific community.

2 Proposed solution and methodology

The work aims at proposing a methodology to help in the model selection decision-making considering different materials. The approach is based on the identifiability analysis [6]. It involves the simulation of adequate mechanical tests for material calibration with perturbations on the material parameters. If the variation in the strain gradients is low when the parameters are perturbed, it means that the calibration of the considered model should be problematic. Therefore, the use of the model is not recommended for the material at hand.

3 Disclamer

The results reflect only the authors' view, and the European Commission is not responsible for any use that may be made of the information it contains.

4 Acknowledgements

This project has received funding from the Research Fund for Coal and Steel under grant agreement No 888153. The authors also acknowledge the financial support under the scope of projects UIDB/00481/2020 and UIDP/00481/2020—FCT—Fundação para a Ciencia e a Tecnologia and CENTRO-01-0145-FEDER022083—Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund. Mariana Conde is grateful to the Portuguese Foundation for Science and Technology (FCT) for the PhD grant 2021.06115.BD.

References

[1] R. J. Nedoushan, *et al.* Simulation of hot forming processes: Using cost effective microstructural constitutive models. Int J of Mech Sc 2014;85:196–204.

[2] Banabic. Advances in anisotropy of plastic behaviour and formability of sheet metals. Int J of Ma 2020;13:749–787

[3] S. Ben-Elechi, *et al.* Sensitivity of friction coefficients, material constitutive laws and yield functions on the accuracy of springback prediction for an automotive part. Int J of Mat For 2021;14:323-340.

[4] S. Kilic, *et al.* Investigation of the Performance of Flow Models for TWIP Steel, J of Mat Eng and Perf 2018;27:4364–4371.

[5] J. Lin, *et al.* Effect of constitutive model on springback prediction of MP980 and AA6022-T4. Int J of Mat For 2020;13:1–13.

[6] Y. Zhang, *et al.* Enhancing the information-richness of specimens for identification of plastic anisotropy through full-field strain fields. Int J of Mech Sc 2021;214:106891.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

The influence of symmetry boundary conditions in the design of heterogeneous mechanical tests using topology optimization

Mafalda Gonçalves*, Sandrine Thuillier† and António Andrade-Campos*

* Centre for Mechanical Technology and Automation (TEMA)
Department of Mechanical Engineering, University of Aveiro
Aveiro, Portugal
e-mail: mafalda.goncalves@ua.pt, gilac@ua.pt

† Univ. Bretagne Sud, UMR CNRS, IRDL
F-56100 Lorient, France
e-mail: sandrine.thuillier@univ-ubs.fr

Abstract: Designing specimens for mechanical testing has gained wide popularity in the material behavior characterization field. Standard mechanical tests are usually performed to extract material properties, however, due to the lack of information provided by each test, mechanical tests with more complex geometries or boundary conditions are being proposed. These present richer mechanical fields and strain and stress states similar to the ones that occur in most common sheet metal forming processes. An efficient way of finding the richest specimen is designing using an optimization approach. In this work, the design by topology optimization is used to find the optimal geometry for the specimen. Given an initial design space with a set of boundary conditions, an adapted version of the theory of compliant mechanisms is employed to obtain the material distribution with the most heterogeneous displacement field. The use of different boundary conditions leads to different material configurations and, therefore, to specimens with different performances. Therefore, this work aims at analyzing the impact of using symmetry boundary conditions in the test design. Several specimen designs are obtained from different initial design domains with and without symmetry boundary conditions. Their influence on the heterogeneity of specimen mechanical fields is then evaluated.

Keywords: Heterogeneous mechanical tests, Material behavior, Topology Optimization, Compliant Mechanisms

1 Introduction

Material behavior characterization and constitutive model calibration are of upmost importance in the development of sheet metal forming parts. In that sense, mechanical tests play a key role in providing information about material behavior, being used to identify material properties. The design of new mechanical tests has been addressed over the years and several designs and methodologies have already been proposed to replace limited standard mechanical tests [1]. Several works have used the heterogeneity of the mechanical fields as a criterion to design a test that provides a high diversity and quality of information [2]. A mechanical test is considered more informative if a large number of mechanical states are covered. The use of an optimization approach is proved to be efficient in finding the specimen design that presents the best quality and quantity of data on the material behavior. The use of topology optimization in the design of tests has already been addressed [3], where the

optimal layout of material for the specimen is found within a given design space. The use of different boundary conditions leads to different material configurations and, therefore, to specimens with different performances. This work aims at studying the influence of symmetry boundary conditions in the design of a heterogeneous mechanical test using topology optimization.

2 Heterogeneous test design

A topology-based optimization methodology is implemented with the aim of finding the material layout for the sheet specimen that corresponds to the test with the best performance. Since inducing heterogeneity directly in the strain field seems to be complex, this methodology proposes to induce heterogeneity through the displacement field. By using an adapted version of the theory of compliant mechanisms, it is possible to apply displacements in specific locations of the specimen and control the displacement field and, consequently, the strain states induced on the specimen [3]. Several specimen geometries with innovative shapes are obtained from different design domains with and without symmetry. Their mechanical fields are then evaluated taking into account the diversity of mechanical phenomena.

3 Disclaimer

The results reflect only the authors' view, and the European Commission is not responsible for any use that may be made of the information it contains.

4 Acknowledgements

This project has received funding from the Research Fund for Coal and Steel under grant agreement No 888153. The authors also acknowledge the financial support under the projects UIDB/00481/2020 and UIDP/00481/2020 – FCT – Fundação para a Ciência e Tecnologia; and CENTRO-01-0145-FEDER-022083 – Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement through the European Regional Development Fund. M. Gonçalves is grateful to the FCT for the Ph.D. grant Ref. UI/BD/151257/2021.

References

[1] Pierron F, Grédiac M. Towards Material Testing 2.0. A review of test design for identification of constitutive parameters from full-field measurements. Strain 2021;57:1–22.

[2] Souto N, Andrade-Campos A, Thuillier S. A numerical methodology to design heterogeneous mechanical tests. Int J Mech Sci 2016;107:264–76.

[3] Gonçalves M, Andrade-Campos A, Barroqueiro B. On the design of mechanical heterogeneous specimens using multilevel topology optimization. Adv Eng Softw 2023;175:103314.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

On the ability of mechanical tests to calibrate anisotropic and rate dependent plasticity models

Thibault Barret*, Miguel Oliveira*†, Antonio Andrade-Campos† and Sandrine Thuilllier*

*Univ. Bretagne Sud,
UMR CNRS 6027,
IRDL, Lorient F-56100, France
e-mail: thibault.barret@univ-ubs.fr sandrine.thuillier@univ-ubs.fr

†Department of Mechanical Engineering
University of Aveiro
Aveiro, Portugal
email: miguel.oliveira@univ-ubs.fr gilac@ua.pt

Abstract: To be able to simulate with precision the sheet metal forming, the input data and particulary the material behavior, numerical models are more and more complex. This complexity has the disadvantage of requiring a lot of experimental data to derive the material parameters. To reduce the number of quasi-homogeneous mechanical tests, a rather recent trend is to use heterogeneous tests, that involve a large distribution of mechanical states. Such an approach is applied to viscoplasticity of a metallic material.

Keywords: heterogeneous tests, plasticity, anisotropy, rate dependent

Metal sheet forming processes such as those used in the automotive industry involve large deformations and viscous phenomena. On the other hand, the numerical simulation of these forming processes has become more and more realistic which requires complex models mixing strain hardening, anisotropy and strain rate sensitivity. The calibration of this type of model is a costly process from a temporal and material point of view if it is carried out only from quasi-homogeneous tests from which only a few parameters are extracted [1].

To answer this new problem, inverse methods such as *Finite Element Model Updating* [2] and *Virtual Fields Method* [3, 4] have appeared and allow to calibrate a multi-parameter model by using all the data offered by the test and the field measurements obtained with digital image correlation. The work now focuses on the geometry of the specimens [5, 6]. Indeed, these new specimens must be able to propose several mechanical states while ensuring not to generate too strong gradients of deformation. Several studies have qualitatively compared these heterogeneous tests in the context of plastic model calibration [7, 8].

This study presents a numerical evaluation of several heterogeneous tests, based on finite element simulations, of their ability to generate the information necessary to calibrate a viscoplastic model for a Dual Phase DP600. An advanced mechanical model is used to take account of anisotropy, hardening and strain rate sensitivity. The corresponding mechanical features are mesured from dedicated experiments. Several indicators are studied such as the equivalent plastic strain and strain rate and the rotation angle. Moreover, the finite element simulation results are used to generate numerically deformed speckle images, also called synthetic images, to model the entire calibration process [9] and evaluate the real ability of the tests to provide the information required to identify the parameters of the viscoplastic model.

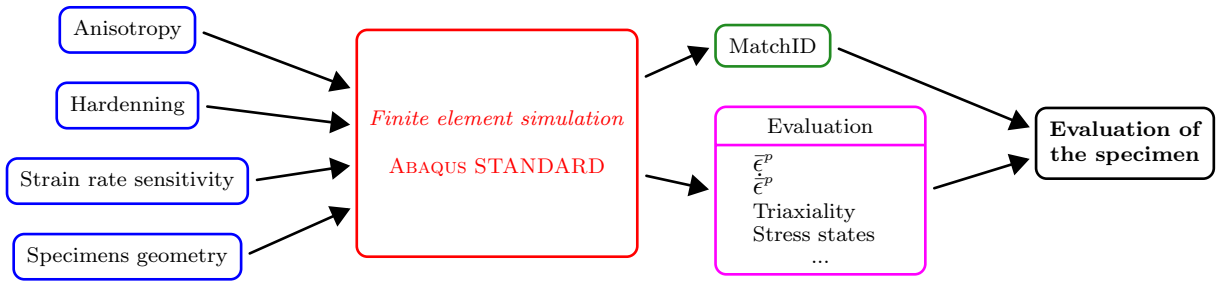


Figure 1: Methodology illustration

Acknowledgements. This study has received funding from the Research Fund for Coal and Steel for the project VForm-xSteels under grant agreement n°888153.

References

[1] Qing Yin et al. "An experimental and numerical investigation of different shear test configurations for sheet metal characterization". *International Journal of Solids and Structures* 51.5 (2014).

[2] Kenneth T. Kavanagh and Ray W. Clough. "Finite element applications in the characterization of elastic solids". *International Journal of Solids and Structures* 7.1 (1971).

[3] Michel Grédiac. "Principe des travaux virtuels et identification". *Comptes rendus de l'Académie des sciences. Série 2, Mécanique, Physique, Chimie, Sciences de l'univers, Sciences de la Terre* 309.1 (1989).

[4] Fabrice Pierron and Michel Grédiac. *The virtual fields method: extracting constitutive mechanical parameters from full-field deformation measurements*. Springer Science & Business Media, 2012.

[5] J-H Kim et al. "Determination of anisotropic plastic constitutive parameters using the virtual fields method". *Experimental Mechanics* 54.7 (2014).

[6] EMC Jones et al. "Parameter covariance and non-uniqueness in material model calibration using the virtual fields method". *Computational Materials Science* 152 (2018).

[7] Miguel G Oliveira, Sandrine Thuillier, and António Andrade-Campos. "Evaluation of heterogeneous mechanical tests for model calibration of sheet metals". *The Journal of Strain Analysis for Engineering Design* 57.3 (2022).

[8] Jean-David Thoby et al. "Robustness of specimen design criteria for identification of anisotropic mechanical behaviour from heterogeneous mechanical fields". *Computational Materials Science* 207 (2022).

[9] Pascal Lava et al. "Validation of finite-element models using full-field experimental data: Levelling finite-element analysis data through a digital image correlation engine". *Strain* 56.4 (2020).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

On the inverse calibration of sheet metal anisotropic plasticity constitutive models using the Arcan test and full-field measurements

João Henriques*, António Andrade-Campos* and José Xavier†

*Centre for Mechanical Technology and Automation (TEMA)
Intelligent Systems Associate Laboratory (LASI)
Department of Mechanical Engineering, University of Aveiro
Aveiro, Portugal
e-mail: joaodiogofh@ua.pt, gilac@ua.pt

†Research and Development Unit for Mechanical and Industrial Engineering (UNIDEMI)
Intelligent Systems Associate Laboratory (LASI)
Department of Mechanical and Industrial Engineering, NOVA School of Science and Technology, NOVA University Lisbon
Lisbon, Portugal
e-mail: jmc.xavier@fct.unl.pt

Abstract: To develop new products, the modern industry relies on simulation tools which use constitutive models and their parameters to predict material mechanical behaviour. With recent technological advancements, it is now possible to measure a variety of strain states using heterogeneous test configurations and full-field measurements. The full-field kinematic data can be coupled with inverse calibration techniques to provide a robust approach for characterising the mechanical behaviour of materials. However, the accuracy of this methodology is influenced by a variety of factors, including the test configuration, the constitutive model and the selection of a suitable identification strategy. In this work, the Arcan mechanical test is used to identify anisotropic plasticity constitutive parameters of sheet metals. Different Arcan test configurations are simulated and analysed using a set of indicators to select the most suitable configuration. To virtually reproduce a real experiment, the computational results are used to numerically deform a speckle pattern image, which is further processed with digital image correlation technique. The full-field measurements are then used for the inverse identification of the constitutive parameters using the virtual fields method.

Keywords: Sheet metal, Anisotropic plasticity, Arcan test, Heterogeneous test evaluation, Inverse identification, Virtual fields method, Digital image correlation.

1 Introduction

Sheet metal part development is becoming more virtual and assisted by the use of numerical simulation. Sheet metal anisotropy is a critical property that has a significant impact on the accuracy of numerical results. Therefore, the quality of the results is strongly dependent on the calibration of the model, which defines the behaviour of the materials during the forming process, including anisotropy. Furthermore, mechanical testing is of utmost importance for the full characterisation of the material mechanical behaviour since the configuration utilised determines the heterogeneity and richness of the information measured. The scientific community has made an increasing effort to develop novel heterogeneous test configurations to replace classical mechanical tests [1], which provide insufficient kinematic data for the full

characterisation of the material behaviour. Moreover, full-field measurements can be coupled with inverse identification techniques [2], such as the virtual fields method (VFM), to fully characterise the material behaviour. This approach uses an optimisation technique to solve a non-direct problem in order to determine the constitutive parameters that best describe the experimental data. This work aims to investigate the use of the Arcan test to identify anisotropic plasticity constitutive parameters of sheet metals through the VFM approach.

2 Inverse identification using the Arcan test

The Arcan test is an interesting test configuration since it allows the loading direction to be varied in a standard uniaxial tensile testing machine. Although some authors used the Arcan test in sheet metal plasticity [3], it is seldom used in heterogeneous test design for the calibration of plastic constitutive models. Nonetheless, the Arcan test has the potential to provide interesting heterogeneous test configurations when used for test design in sheet metal plasticity. Several Arcan test configurations are simulated and further evaluated regarding their mechanical state heterogeneity using a set of indicators. The numerical results are then used to generate synthetically deformed speckle pattern images which are processed by digital image correlation (DIC). This kinematic data is then used for the inverse calibration of the sheet metal constitutive parameters using the VFM.

3 Acknowledgements

J. Henriques is grateful to the Portuguese Foundation for Science and Technology (FCT) for the Ph.D. grant 2021.05692.BD. This project has received funding from the Research Fund for Coal and Steel under grant agreement No 888153. The authors gratefully acknowledge the financial support of the FCT under the project PTDC/EMEAPL/29713/2017 by UE/FEDER through the programs CENTRO 2020 and COMPETE 2020, and UID/EMS/00481/2013-FCT under CENTRO-01–0145-FEDER-022083. Authors also acknowledge the FCT (FCT - MCTES) for its financial support via the projects UIDB/00667/2020 (UNIDEMI).

4 Disclaimer

The results reflect only the authors' view, and the European Commission is not responsible for any use that may be made of the information it contains.

References

[1] Pierron F, Grédiac M. Towards Material Testing 2.0. A review of test design for identification of constitutive parameters from full-field measurements. Strain 2021; 57:e12370.

[2] Henriques J, Conde M, Andrade-Campos A, Xavier J. Identification of Swift Law Parameters Using FEMU by a Synthetic Image DIC-Based Approach. Key Eng. Mater. 2022; 926:2211–2221.

[3] Kumar A, Singha M K, Tiwari V. Structural response of metal sheets under combined shear and tension. Structures 2020; 26:915–933.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

IDENTIFICATION OF THROUGH-THICKNESS WORK HARDENING VARIATION OF THICK HIGH STRENGTH STEEL USING THE VIRTUAL FIELD METHOD

Alessandro Lambrughi[1], Steven Cooreman[3] , Sandrine Thuillier[2] and Sam Coppieters[1]

[1] Department of Materials Engineering, KU Leuven,
Gent Technology Campus, Belgium
e-mail: alessandro.lambrughi@kuleuven.be and sam.coppieters@kuleuven.be

[2] Univ. Bretagne Sud, UMR CNRS 6027, IRDL, Lorient F-56100, France
e-mail: sandrine.thuillier@univ-ubs.fr

[3] ArcelorMittal Global R&D / OCAS NV
Zelzate , Belgium
e-mail: steven.cooreman@arcelormittal.com

Abstract: Heavy gauge high strength steels produced by thermomechanical controlled processing often exhibit a gradient of mechanical properties through the thickness. Moreover, the ductility beyond the point of uniform elongation and the associated post-necking region is sensitive to the sample thickness. Both effects have a relevant impact on the plastic material behavior during forming operations. Therefore, a reliable forming simulation based on a finite element analysis must account for these effects through a constitutive plasticity model calibrated with customized experimental tests. This work proposes an inverse characterization of the through-thickness material properties of a thick S700MC high strength steel. To this end, the thick tensile test sample is sliced into several thin tensile test samples. Standard tensile tests, augmented with Digital Image Correlation (DIC), on these samples reveal the variation of work hardening at relatively small plastic strains. Therefore, the Virtual Fields Method (VFM) is used to extend the validity of the standard tensile test and extract the post-necking work hardening variation in the through-thickness direction.

Keywords: S700MC, Through-thickness properties, Digital Image Correlation, Inverse identification, Virtual Field Method

1. Introduction

Since the earliest developments in the 1960s, thermomechanical controlled processing (TMCP) is broadly used by many steelmaking companies to manufacture high-strength steels aimed for structural applications such as pipe lines for gas transportation, motor vehicles or maritime applications [1] [2]. These procedures rely on a combination of controlled hot rolling and accelerated cooling operations allowing to produce a material having higher strength, toughness and weldability compared to conventionally hot rolled steels [1] [3]. The properties enhancement is mainly based on a microstructural refinement and transformation. Nevertheless, in TMCP, the improvement of the mechanical characteristics is accompanied by a rise of their anisotropy through the thickness. This gradient in properties occurs because a heterogeneous microstructure through the sheet thickness is formed. Indeed, as shown in [2], [3] and [4], the microstructure of the surface layers is generally finer and with less inclusions with respect to the central layer. Moreover, in the central region, a segregation band with an inhomogeneous chemical composition of the alloying elements often appears. The reason inducing all these differences in the microstructure is related to the non-homogeneous cooling rate between surface and center of the plate during TMCP. In addition to the through-thickness properties variation, another factor influencing the structural performance of a high-strength steel sheet is the sample thickness. The formability expressed in terms of ductility measured in a standard tensile test shows a thickness dependency. Generally, thicker samples present a higher ductility while thinner ones are more brittle as shown in [5] for structural high-strength steels and in [6] and [7] for other metals such as copper and aluminium. For high-strength steels, this ductility discrepancy is mainly related to the post-necking characteristics of the material. In fact, an increase of the thickness leads to larger post-necking elongations compared to thin samples [5].

Numerical simulation based on the finite element method are nowadays commonly used for industrial forming processes in the frameworks of process optimization and structural integrity analysis. The accuracy of the simulation results highly depends on the material response described with the constitutive plasticity model. For this reason, effects such as the gradient of mechanical properties through the thickness have to be characterized

so that a trustworthy material model can be established. This work aims at an inverse characterization of the through-thickness work hardening variation at large plastic strains.

2. Methodology: experimental Setup and tested Samples

The methodology used in this work to investigate the above-mentioned material characteristics consists of conducting several mechanical quasi-static standard tensile tests on dog bone specimens. In order to investigate the through-thickness work hardening variation, the thick tensile sample is sliced into thin tensile samples using wire cut Electrical Discharge Machining (EDM) (Figure 1). The identification of the work hardening behavior was performed through a full-field measurement technique and the VFM. Digital image correlation (DIC) with two stereo configurations (4 cameras) measuring front and back surface of the sample simultaneously was employed to measure the inhomogeneous surface strain during post-necking stage (Figure 2).

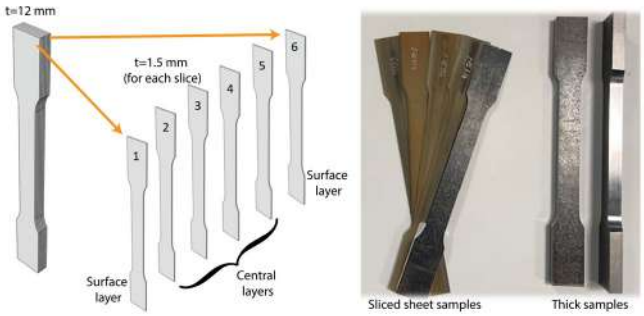


Figure 1 Illustration of the samples used for experimental characterization: thick and sliced sheet samples

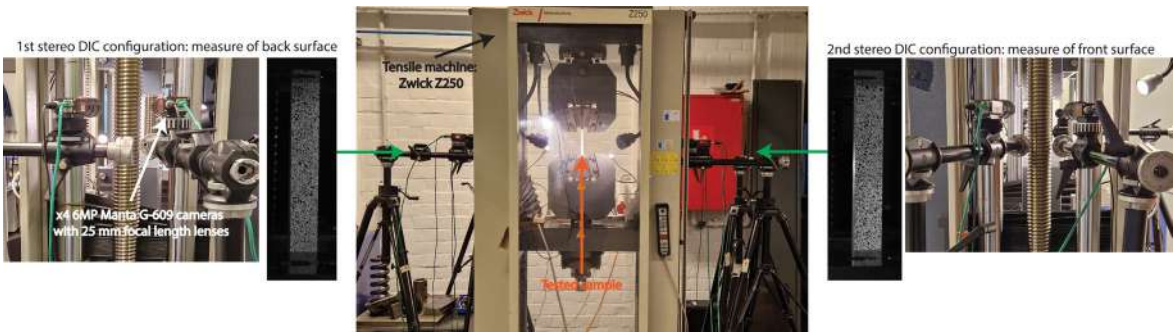


Figure 2 Illustration of the DIC experimental setup: 2 stereo configurations were used simultaneously

Acknowledgements

This project has received funding from the Research Fund for Coal and Steel under grant agreement No 888153.

References

[1]. Imao Tamura, Hiroshi Sekine, Tomo Tanaka and Chiaki Ouchi, Thermomechanical Processing of High-strength Low-alloy Steels. UK: Butterworths; 1988. Chapters 1 and 5

[2]. Bertolo, V.M., Jiang, Q., Walters, C.L., Popovich, V.A., Effect of Microstructure on Cleavage Fracture of Thick-Section Quenched and Tempered S690 High-Strength Steel. In: Characterizaton of minerals, metals and materials 2020, p155-168 (2020)

[3]. Chiaki Ouchi, Development of Steel Plates by Intensive Use of TMCP and Direct Quenching Processes, ISIJ International, vol 41, p542-553 (2001)

[4]. Virginia Bertolo et al., A comprehensive quantitative characterization of the multiphase microstructure of a thick-section high strength steel, Journal of Materials Science, vol 57, p7101-7126 (2022)

[5]. W.J. Yuan et al., Influence of specimen thickness with rectangular cross-section on the tensile properties of structural steels, Materials Science and Engineering A, vol 532, p601-605 (2012)

[6]. Y.H. Zhao et al., Influence of specimen dimensions on the tensile behavior of ultrafine-grained Cu, Scripta Materialia, vol 59, p627-630 (2008)

[7]. Chang Hee Suh, Effects of thickness and surface roughness on mechanical properties of aluminum sheets, Journal of Mechanical Science and Technology, vol 24, p2091-2098 (2010)

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

On the constraints and consistency in implicit elastoplastic constitutive modelling using ANNs and indirect training

Rúben Lourenço[*,1], **Elías Cueto**[†], **Pétia Georgieva**[**] **and A. Andrade-Campos**[‡,2]

[*,‡] Dept. of Mechanical Engineering (DEM)
Centre for Mechanical Technology and Automation (TEMA),
Intelligent Systems Associate Laboratory (LASI), University of Aveiro
Aveiro, Portugal
e-mail: [1]rubenl@ua.pt, [2]gilac@ua.pt

[†] Aragon Institute of Engineering Research (I3A)
University of Zaragoza
Zaragoza, Spain
e-mail: becueto@unizar.es

[**] Institute of Electronics and Informatics Engineering of Aveiro (IEETA)
Dep. of Electronics, Telecommunications and Informatics, University of Aveiro
Aveiro, Portugal
e-mail: petia@ua.pt

Abstract: The training of an Artificial Neural Network (ANN) for implicit constitutive modelling mostly relies on labelled data pairs, however, some variables cannot be physically measured in real experiments. As such, the training should preferably be carried out indirectly, making use of experimentally measurable variables. The unconstrained training of an ANN's parameters often leads to spurious responses that do not comply with the physics of the problem. Applying constraints during training ensures not only the physical meaning of the ANN predictions but also potentially increases the convergence to a global minimum, while improving the model's performance. An ANN material model is trained using a novel indirect approach, where the local and global equilibrium conditions are ensured employing the Virtual Fields Method (VFM). Examples of physical constraints are analyzed and applied during the training process.

Keywords: Constitutive model, Elastoplasticity, Neural network, Indirect training, Constrained optimization

1 Introduction

ANNs are powerful function approximators that can be used to learn constitutive relationships directly from data [1]. In general, training relies on labelled data pairs, usually stress-strain, obtained from numerically generated datasets. Nevertheless, in a real experiment certain variables (e.g. stress) are not measurable, thus the training should be carried out indirectly using experimentally measurable variables only.

A standard ANN is a black-box model in which its structure is not easily interpretable and there is no guarantee that its predictions are usable, as they can violate fundamental laws of mechanics and thermodynamics [1]. Therefore, it is important to enforce physics-based constraints when using ANNs for implicit constitutive modelling, similarly to Physical Informed Neural Networks (PINNs). These constraints act as a regularization agent for

ANNs, reducing the space of admissible solutions and allowing the network to learn with smaller datasets [2].

The VFM, first introduced by Grédiac [3], is a state-of-the-art method employed in the identification of constitutive parameters. The key elements behind the VFM are the Principle of Virtual Work (PVW) and the choice of virtual fields. According to the PVW, the internal virtual work must be equal to the external virtual work performed by the external forces [4]. The virtual fields consist of virtual strains, $\boldsymbol{\varepsilon}^*$, and virtual displacements, $\mathbf{u}^*$, defined independently of the measured displacements/strains.

In the present work, ANN models are used to learn constitutive behavior of a virtual material. A novel indirect training methodology employing the sensitivity-based Virtual Field Method (VFM) [4] is used to train the models and study the influence of applying constraints during training.

2 Disclaimer

The results reflect only the authors' view, and the European Commission is not responsible for any use that may be made of the information it contains.

3 Acknowledgements

Rúben Lourenço acknowledges the Portuguese Foundation for Science and Technology (FCT) for support from grant 2020.05279.BD, co-financed by the European Social Fund, through the programme CENTRO 2020. The authors also acknowledge the financial support of FCT under the projects UID/EMS/00481/2013-FCT through CENTRO-01-0145-FEDER-022083. This project is also supported by the Research Fund for Coal and Steel under grant agreement No 888153.

References

[1] K. Linka, E. Kuhl, W. Ehlers, M. Itskov, C. Miehe, M. Ortiz, J. Schröder, E. Stein, and P. Steinmann, "A new family of constitutive artificial neural networks towards automated model discovery," 9 2022.

[2] F. Masi, I. Stefanou, P. Vannucci, and V. Maffi-Berthier, "Thermodynamics-based artificial neural networks for constitutive modeling," *Journal of the Mechanics and Physics of Solids*, vol. 147, p. 104277, 2 2021.

[3] M. Grédiac, "Principe des travaux virtuels et identification," *Comptes Rendus de l'Académie des Sciences*, vol. 309, pp. 1–5, 1989.

[4] A. Marek, F. M. Davis, and F. Pierron, "Sensitivity-based virtual fields for the non-linear virtual fields method," *Computational Mechanics*, vol. 60, pp. 409–431, 2017.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Analysis of Creep in Composites with the Scaled Boundary Finite Element Method

Johanna Eisenträger[1,*], Junqi Zhang[2], Sascha Eisenträger[3] and Chongmin Song[4]

[1,*] Otto von Guericke University Magdeburg
Magdeburg, Germany
e-mail: johanna.eisentraeger@ovgu.de

[2] Beijing University of Technology
Beijing, PR China
e-mail: zhangjunqi@bjut.edu.cn

[3] Technical University of Darmstadt
Darmstadt, Germany
e-mail: sascha.eisentraeger@tu-darmstadt.de

[4] University of New South Wales Sydney
Sydney, Australia
e-mail: c.song@unsw.edu.au

Abstract: Nowadays, composites consisting of a matrix with inclusions of arbitrary shapes and distribution have found widespread applications. Since the macroscopic behaviour of composite structures is determined by the microstructure, simulation of large-scale problems remains a major challenge, which is addressed by the contribution at hand. To this end, we make use of the scaled boundary finite element method (SBFEM), which is ideally suited to be combined with a quadtree-based meshing procedure due to its flexibility with respect to element shapes. This procedure allows for an automatic and fast discretization of microstructural images. Because many matrix materials suffer from creep, we present the implementation of a non-linear constitutive model for rate-dependent inelasticity into the SBFEM. In order to increase the numerical efficiency and simplify the formulation, the stress update algorithm is only performed at the scaling centre of the polytope elements. Furthermore, to demonstrate the straightforward application of the proposed framework, a creep test of a metal-matrix composite is simulated. While the inclusions are assumed to deform only elastically, rate-dependent inelasticity is taken into account to model the mechanical behaviour of the matrix. The spatial discretization is generated from a microstructural image such that one is enabled to obtain detailed stress and strain fields in the analysis.

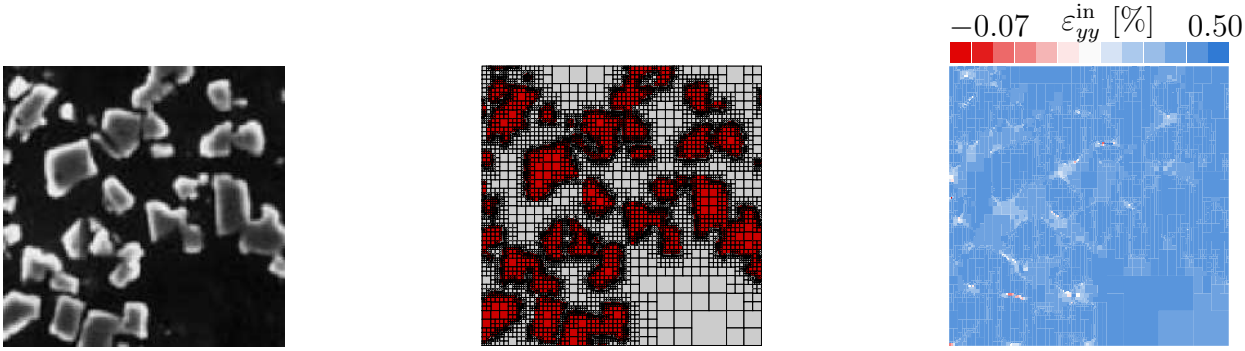
Keywords: Creep, Composites, SBFEM, Image-Based Analysis

1 Introduction

The current contribution presents an approach to model the inelastic behaviour of composites consisting of a matrix with inclusions of arbitrary shape and distribution. We make use of the scaled boundary finite element method (SBFEM), which has first been proposed in Ref. [1]. Since it is straightforward to construct polytope elements in the SBFEM because of its flexibility with respect to the element shapes, we combine the SBFEM with a quadtree-based meshing paradigm for discretization of microstructural images.

2 Rate-Dependent Inelasticity in a Metal-Matrix Composite

This section briefly summarises the simulation of a creep test of a metal-matrix composite based on the SBFEM. The implementation of non-linear constitutive models for rate-dependent inelasticity into the SBFEM is based upon the principle of virtual work, which is explained in detail in Ref. [3]. In analogy to the FEM, the use of an inelastic material model requires the computation of the current stresses and the consistent tangent operator, which is done based on a stress update algorithm. Note that in order to increase numerical efficiency, the stress update algorithm is only performed at the scaling centre of each element. Further information on the employed meshing approach can be found in Ref. [2]. Exemplarily, Fig. 1 presents some results of an analysis of a metal-matrix composite (MMC). While the aggregates are assumed to behave linear elastically, creep is modelled within the matrix. In the detailed contour plot of the inelastic strain (Fig. 1c), one observes localisations in the matrix near the interfaces of the aggregates.



(a) Micrograph. (b) Quadtree mesh. (c) Vertical inel. strain.

Figure 1: Micrograph, quadtree mesh, and contour plot of vertical inelastic strain of a ferrous-based MMC with tungsten carbide, cf. [3].

3 Acknowledgements

Johanna Eisenträger acknowledges the funding by the German Research Foundation (Deutsche Forschungsgemeinschaft - DFG) in context of the Project 422068083.

References

[1] Song C, Wolf JP. The scaled boundary finite-element method—alias consistent infinitesimal finite-element cell method—for elastodynamics. Comput Methods in Appl Mech Eng 1997;147:329–355.

[2] Zhang J, Eisenträger J, Duczek S, Song C. Discrete modeling of fiber reinforced composites using the scaled boundary finite element method. Compos Struct 2019;235:111744.

[3] Eisenträger J, Zhang J, Song C, Eisenträger S. An SBFEM Approach for Rate-Dependent Inelasticity with Application to Image-Based Analysis. Compos Struct 2020;182:105778.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Multiscale modeling of heterogeneous structures based on a localized model order reduction approach

P. Diercks*, A. Robens-Radermacher*, K. Veroy† and J. F. Unger*

* Bundesanstalt für Materialforschung und -prüfung (BAM)
Unter den Eichen 87
12205 Berlin
{philipp.diercks, annika.robens-radermacher, joerg.unger}@bam.de

† Centre for Analysis, Scientific Computing and Applications (CASA)
Department of Mathematics and Computer Science, TU Eindhoven
P.O. Box 513, 5600 MB Eindhoven, The Netherlands
k.p.veroy@tue.nl

Abstract: Many of today's problems in engineering demand reliable and accurate prediction of failure mechanisms of mechanical structures. Thus, it is necessary to take into account the heterogeneous structure on the smaller scale, to capture the underlying physical phenomena. However, this poses a great challenge to the numerical solution since the computational cost is significantly increased by resolving the smaller scale in the model. Moreover, in applications where scale separation as the basis of classical homogenization schemes does not hold, the influence of the smaller scale on the larger scale has to be modelled directly.

This work aims to develop an efficient concurrent methodology to model heterogeneous structures combining the variational multiscale method (VMM) [1] and model order reduction techniques (e. g. [2]). First, the influence of the smaller scale on the larger scale can be taken into account following the additive split of the displacement field as in the VMM. Here, also a decomposition of the global domain into subdomains, each containing a fine grid discretization of the smaller scale, is introduced. Second, local reduced approximation spaces for the smaller scale solution are constructed by exploring possible solutions for each subdomain based on the concept of oversampling [3]. The associated transfer operator is approximated by random sampling [4]. Herein, we propose to incorporate the actual physical behaviour of the structure of interest in the training data by drawing random samples from a multivariate normal distribution with the solution of a reduced global problem as mean. The local reduced spaces are designed such that local contributions of each subdomain can be coupled in a conforming way. Thus, the resulting global system is sparse and reduced in size compared to the direct numerical simulation, leading to a faster solution of the problem.

The authors gratefully acknowledge financial support by the German Research Foundation (DFG), project number 394350870, and by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC Grant agreement No. 818473).

Keywords: Multiscale Method, Variational Multiscale Method, Domain Decomposition, Model Order Reduction

References

[1] Thomas J.R. Hughes, Gonzalo R. Feijóo, Luca Mazzei, and Jean-Baptiste Quincy. The variational multiscale method—a paradigm for computational mechanics. *Comput. Method. Appl. M.*, 166(1-2):3–24, November 1998.

[2] Jan S Hesthaven, Gianluigi Rozza, and Benjamin Stamm. *Certified Reduced Basis Methods for Parametrized Partial Differential Equations.* SpringerBriefs in Mathematics. Springer International Publishing, 2016.

[3] Thomas Y. Hou and Xiao-Hui Wu. A multiscale finite element method for elliptic problems in composite materials and porous media. *J. Comput. Phys.*, 134(1):169–189, June 1997.

[4] Andreas Buhr and Kathrin Smetana. Randomized local model order reduction. *SIAM J. Sci. Comput.*, 40(4):A2120–A2151, January 2018.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Computational modelling of stress gradient continua

Tobias Kaiser*, Samuel Forest† and Andreas Menzel‡

*Institute of Mechanics, TU Dortmund University, Dortmund, Germany
Mechanics of Materials Group, Eindhoven University of Technology, Eindhoven, The Netherlands
e-mail: tobias.kaiser@tu-dortmund.de

†Centre des Matériaux, MINES ParisTech, PSL University, Paris, France
e-mail: samuel.forest@mines-paristech.fr

‡Institute of Mechanics, TU Dortmund University, Dortmund, Germany
Division of Solid Mechanics, Lund University, Lund, Sweden
e-mail: andreas.menzel@tu-dortmund.de

Abstract: Dating back to the pioneering works by Mindlin almost 60 years ago, strain gradient approaches are nowadays well-established. Stress gradient approaches as their counterpart have, however, only recently been proposed and have since been in the focus of intense research. Although existence and uniqueness theorems for stress gradient problems have been established, the study of stress gradient continua is, today, limited to a restricted class of boundary value problems for which analytical solutions can be furnished. Against this background, a finite element implementation of the stress gradient theory is proposed in this work. Tension and torsion problems are considered for which analytical solutions can be derived for validation purposes. Particular focus is laid on the boundary conditions since the stress gradient theory requires not only the tractions but rather the complete stress tensor to be prescribed at the boundaries. The natural occurrence of an internal length scale and the associated smaller-is-softer-type size effect are discussed.

Keywords: Stress gradient theory, Size effects, Stress-free boundary layer, Finite elements

1 Introduction

The stress gradient theory is a novel modelling approach to account for the underlying material microstructure in macroscopic simulations [1]. It is based on the introduction of additional degrees of freedom, so-called micro-displacements, that characterise the deformation of the microstructure and occur as energetic duals to the stress gradient in the generalised work of internal forces. In particular, it has been revealed in [3] that, by using an extended homogenisation approach, the micro-displacements can be related to the first moment of the microscale strain field. The formulation has been shown to be well-posed in the sense that existence and uniqueness theorems can be established provided that suitable boundary conditions are prescribed [2]. Motivated by these developments and driven by the desire to study general boundary value problems of stress gradient continua, a finite element implementation of the stress gradient theory was recently proposed in [4].

2 Stress gradient theory

At the outset of the developments, a functional dependency of the generalised stress energy density function $w^*\left(\boldsymbol{\sigma}, \boldsymbol{R}\right)$ on the small deformation stress tensor $\boldsymbol{\sigma}$ and the hyperstress tensor

$\boldsymbol{R}$ is assumed, and the generalised set of static admissibility conditions

$$\nabla \cdot \boldsymbol{\sigma} = \boldsymbol{0} \quad \text{on } \mathcal{B}\,, \tag{1a}$$

$$\boldsymbol{R} - [\nabla \boldsymbol{\sigma}]^{\text{dev}} = \boldsymbol{0} \quad \text{on } \mathcal{B}\,, \tag{1b}$$

is postulated. By multiplying (1) with virtual displacements $\delta\boldsymbol{u}$ and virtual micro-displacements $\delta\boldsymbol{\Phi}$, by integration the ensuing equation over domain $\mathcal{B}$ and by making use of Gauss's theorem one arrives at the generalised virtual work statement

$$\int_{\mathcal{B}} \boldsymbol{\sigma} : [[\nabla \delta\boldsymbol{u}]^{\text{sym}} + \nabla \cdot \delta\boldsymbol{\Phi}] + \boldsymbol{R} \therefore \delta\boldsymbol{\Phi} \, \mathrm{d}v = \int_{\partial\mathcal{B}} \boldsymbol{\sigma} : [[\delta\boldsymbol{u} \otimes \boldsymbol{n}]^{\text{sym}} + \delta\boldsymbol{\Phi} \cdot \boldsymbol{n}] \, \mathrm{d}a \quad . \tag{2}$$

Equation (2) suggests energetic dualities between the stress tensor and the generalised strain tensor $\boldsymbol{e} = [\nabla \boldsymbol{u}]^{\text{sym}} + \nabla \cdot \boldsymbol{\Phi}$, and between the hyperstress tensor and the micro-displacement field. Moreover, the latter observation motivates the introduction of the generalised strain energy density function $w(\boldsymbol{e}, \boldsymbol{\Phi})$ such that

$$\boldsymbol{\sigma} = \frac{\partial w(\boldsymbol{e}, \boldsymbol{\Phi})}{\partial \boldsymbol{e}} \quad , \tag{3a}$$

$$\boldsymbol{R} = \frac{\partial w(\boldsymbol{e}, \boldsymbol{\Phi})}{\partial \boldsymbol{\Phi}} \quad , \tag{3b}$$

hold. By introducing the third-order tensor field $\boldsymbol{\Psi} = \boldsymbol{\Psi}^{\text{dev}} + \boldsymbol{\Psi}^{\text{sph}}$, hereafter referred to as the generalised displacement field, with

$$\boldsymbol{\Psi}^{\text{dev}} = \boldsymbol{\Phi} \quad , \tag{4a}$$

$$\boldsymbol{\Psi}^{\text{sph}} = \frac{1}{2} [\boldsymbol{u} \otimes \boldsymbol{I} + \boldsymbol{u} \overline{\otimes} \boldsymbol{I}] \quad , \tag{4b}$$

the virtual work statement (3) can be recast in the form

$$\int_{\mathcal{B}} \boldsymbol{\sigma} : [\nabla \cdot \delta\boldsymbol{\Psi}] + \boldsymbol{R} \therefore \delta\boldsymbol{\Psi} \, \mathrm{d}v = \int_{\partial\mathcal{B}} \boldsymbol{\sigma} : \delta\boldsymbol{\Psi} \cdot \boldsymbol{n} \, \mathrm{d}a \quad . \tag{5}$$

3 Finite element implementation

The virtual work statement (5) serves as the basis for the finite element implementation proposed in [4]. In particular, it is noted that the boundary term on the right-hand side implies that either the normal projection of the generalised displacement field or the complete stress tensor can independently be prescribed at the boundary. This allows, amongst others, the study of stress-free boundary layer effects.

References

[1] Forest S, Sab K. Stress gradient continuum theory. Mech Res Commun 2012;40:16–25, doi: 10.1016/j.mechrescom.2011.12.002

[2] Sab K, Legoll F, Forest S. Stress gradient elasticity theory: Existence and uniqueness of solution. J Elast 2016;123(2):179–201, doi: 10.1007/s10659-015-9554-1

[3] Hütter G, Sab K, Forest S. Kinematics and constitutive relations in the stress-gradient theory: interpretation by homogenization. Int J Solid Struct 2020;193–194:90–97, doi: 10.1016/j.ijsolstr.2020.02.014

[4] Kaiser T, Forest S, Menzel A. A finite element implementation of the stress gradient theory. Meccanica 2021;56:1109–1128, doi: 10.1007/s11012-020-01266-3

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

How to integrate Galerkin weak forms during preprocessing

Bode, Tobias[*] [†]

[*] Institute of Continuum Mechanics
Leibniz University Hannover
Garbsen, Germany
e-mail: bode@ikm.uni-hannover.de

[†] Cluster of Excellence PhoenixD
Leibniz University Hannover
Hannover, Germany

Abstract: Modeling for the description and prediction of processes in nature often leads to partial differential equations. Solving these field equations can only be done analytically in very few cases, so that in practice numerical approximation methods are often used. Variational methods like the Galerkin method have proven to be very effective and are widely used in industry and research. To set up the system of equations, integration over the area to be calculated is necessary. For more complex geometries or nonlinear equations, analytical integration becomes difficult or even infeasible, so that integration is also often performed numerically in the form of weighted evaluations of the integrand, the Gauss quadrature. In order to benefit from the quasi-optimal accuracy of the Galerkin method according to Cea's lemma in the linear case, the quadrature scheme must also be of sufficient accuracy. On the contrary, for more complex constitutive laws, under-integration is often used in engineering to save computational time. On the example of the principle of virtual work, the lecture shall demonstrate a pre-processing method, how specific approximations of the integrand help that only one integration point is needed in the analysis phase without suffering a loss of geometrical accuracy even for high-order elements. Thereby, the integration weights of this point become independent of the primary variables and can thus be calculated during preprocessing.

Keywords: Numerical Integration, One-Point Quadrature, Galerkin Methods

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Buckling analysis of a beam made of Gyroid cells

Donato D'Aprile[a], Simone Morganti[b], Arsenio Cutolo[c], Massimiliano Fraldi[c], Ferdinando Auricchio[a]

[a] Department of Civil Engineering and Architecture
University of Pavia,
Pavia, Italy

[b] Department of Electrical, Computer, and Biomedical Engineering
University of Pavia,
Pavia, Italy

[c] Department of Structures for Engineering and Architecture
University of Naples Federico II,
Naples, Italy

Abstract: In the last few years, an increasing attention has been paid to metamaterials, materials with internal structures, usually organized in repeated patterns and with properties directly derived from the specific design. In this scenario, Triply Periodic Minimal Surfaces (TPMS) represent a fascinating family of cellular structured materials that can be precisely described by trigonometric equations in a three-dimensional space [1]. Among the available TPMS, we focus on the Gyroid. The Gyroid surface has no planes of symmetry and no embedded straight lines, and revealed to have interesting geometrical and mechanical properties [2]. In particular, in this work, we consider a beam made of repetition of Gyroid cells, and we investigate its instability behaviour. First, we conduct a geometrical analysis on a single Gyroid cell to study the variation of the inertia and area along the beam axial direction. Then, we present buckling analyses of the beam performed with Abaqus software. The results reveal a remarkable lower value of the critical load than the one obtained using the classical Euler beam equations, taking a constant inertia equal to the minimum value of the varying axially inertia of the Gyroid beam. For this reason, we finally solve the Euler's Elastica equation in Matlab for a simplified 1D-problem of a beam with variable inertia. The results show that the beam variable inertia and its axial deformation play a key role in determining the critical load.

Keywords: Triply Periodic Minimal Surfaces, Gyroid, Inertia, Instability, Euler's Elastica

References

[1] Ramírez, E. A., et al. Design parameters effects on relative density of triply periodic minimal surfaces for additive manufacturing. Procedia CIRP, 2021, 100: 13-18.

[2] Abueidda, Diab W., et al. Mechanical properties of 3D printed polymeric Gyroid cellular structures: Experimental and finite element study. Materials & Design, 2019, 165: 107597.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Failure by design of architected interfaces: Towards a unified theory for elastic foundations

Adrianos E. F. Athanasiadis[*1], Michal K. Budzik[†], Dilum N. Fernando[*], Marcelo A. Dias[*2]

[*] Institute of Infrastructure and Environment (IIE)
School of Engineering, The University of Edinburgh, Edinburgh, United Kingdom
e-mails: [1] a.athanasiadis@ed.ac.uk, [2] marcelo.dias@ed.ac.uk

[†] Laboratory for Mechanics and Physics of Solids (LAMPS)
Department of Mechanical and Production Engineering, Aarhus University, Aarhus, Denmark

Abstract: In this work, we investigate the mechanical properties of conceptual structural adhesive joints, in which the role of the adhesive is played by an architected interface. In contrast to isotropic and homogeneous interfaces, properties of architected interfaces are controlled by tailoring the microstructure. Therefore, we augment existing theoretical frameworks by providing efficient homogenised models based on Cosserat elasticity, which accounts for emerging micromechanical effects. By using such homogenisation procedures, we demonstrate how characteristic lengths govern the mode I fracture behavior of architected interfaces. It is revealed that interactions amongst lengths-scales originating from microstructure allow control of the characteristic fracture process zone size. The findings are compared against numerical simulations justifying the effectiveness of the method. The theoretical and numerical approaches are inter-winded, revealing a set of critical parameters that need to be considered when designing architected interfaces under failure loads.

Keywords: Architected Materials, Adhesive Joints, Metamaterials, Micropolar, Cosserat Elasticity

1 Introduction

In the fast-growing industrial sectors for infrastructure engineering, such as transportation and energy, drives for efficiency and functionality inevitably rely on our understanding of confined materials and adhesive joints [1]. In that regard, an important contribution has been made towards exploring the fabrication and static properties of simple lattice structures, against the more often used foams or honeycomb cell cores [2]. Bondlines are used and designed to ensure structural integrity and maximise efficiency of load transfer between joined materials. With emerging additive manufacturing technologies, our focus turns into architected interfaces with the scope of merging mechanical metamaterials into conceptual joint designs. We introduce a new concept of low-density interfaces with properties that could be carefully tailored along multiple directions and critical load localisations.

2 The need for augmenting the existing theory

In our recent work [3] we showcased how lattices length-scales and the level of confinement of architected materials affect the fracture process zone in mode I loading—analytical and numerical methods are presented in the context the double cantilever beam configuration. However, modeling of architected structures is a daunting task that relies significantly on

homogenisation procedures. Hence, in our model, the architected interface was treated as a homogeneous elastic foundation. In principle, architected materials can experience large overall deformations caused by localised rotations, i.e. microrotations that produce couple stress reactions to the joined materials. Therefore, in this context, the classical theory of elastic foundation, which is used extensively in failure problems, does not yield the required accuracy. In this work, we augment the concept of elastic foundation accounting for micromechanical effects by using the theory of micropolar elasticity [4], in order to reduce modeling complexity aiming to arrive at closed-form solutions for specific failure problems.

3 The resulting parametric space

The theory of micropolar elasticity is able to capture effectively architected materials that undergo local rotations, namely bending-dominated structures, auxetic foams, trusses, and grids [5, 6], by considering additional effective material properties as functions of the respective microstructure. In line with [7, 4], we utilise appropriate stress functions to solve the compatibility equations and obtain the stress, couple stress, displacement, and microrotation fields. This approach allows us to calculate the effective linear stiffness as well as an additional rotational stiffness of the foundation accounting for micropolarity. Therefore, in addition to the usual parameters of the problem (Young's modulus, Poisson's ratio, and thickness), our model considers two additional parameters that govern the micropolar behaviour of an effective bulk that emerges from the lattice. Namely, the characteristic length for bending, measuring the material's resistance to (micro)bending, and the coupling number, characterising the coupling between linear and rotational elastic fields. Such consideration significantly expands the available parametric space, which can lead to new material configurations worth investigating. The findings are then compared to numerical simulations revealing how each length-scale affects the behaviour, and proving the method's accuracy.

References

[1] Zuo P. and Vassilopoulos A.P. Review of fatigue of bulk structural adhesives and thick adhesive joints. Int. Mater. Rev. (2020).

[2] Wadley H.N., Fleck N.A. and Evans A.G. Fabrication and structural performance of periodic cellular metal sandwich structures. Compos. Sci. Technol., 63 (16) (2003).

[3] Athanasiadis A.E.F., Dias M.A. and Budzik M.K. Can confined mechanical metamaterials replace adhesives? Extr. Mech. Lett., 48 (2021).

[4] Nowacki W. Theory of Asymmetric Elasticity. Polish Scientific Publishers; 1986.

[5] Lakes R. Experimental Micro Mechanics Methods for Conventional and Negative Poisson's Ratio Cellular Solids as Cosserat Continua. J. Eng. Mat. Tech., 113 (1) (1991).

[6] Bažant Z.P., Christensen M. Analogy between micropolar continuum and grid frameworks under initial stress. Int. J. Solids Struct., 8 (1972).

[7] Allen H.G. Analysis and design of structural sandwich panels. Pergamon Press; 1969.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Dynamic multifield continualization method for magneto-electro-elastic layered periodic materials

Rosaria Del Toro*, Maria Laura De Bellis* and Andrea Bacigalupo†

* Department INGEO, University of Chieti-Pescara, Pescara, Italy
e-mail: rosaria.deltoro@unich.it marialaura.debellis@unich.it

† Department DICCA, University of Genova, Genova, Italy
e-mail: andrea.bacigalupo@unige.it

Abstract: Magneto-electro-elastic (MEE) layered periodic materials are a topic of great interest due to their challenging applications in many industrial fields. In this work, field equations governing a MEE layered periodic material are proposed and a complex notation for the unknown variables is introduced. Then, a dynamic multifield continualization method is outlined to analyze MEE wave propagation traveling along the orthogonal direction to the material layering by matching the $\mathcal{Z}$-transform of the vector collecting the nodal fields to the two-sided Laplace transform of the same vector at the macroscale. The continualization technique allows identifying multifield integral-type non-local continua and multi-field generalized gradient-type (higher-order) non-local continua. Finally, to test the accuracy of the proposed approach, the complex spectra derived from the continualization technique are compared with those provided by the Floquet-Bloch theory.

Keywords: Periodic MEE materials, Transfer Matrix, Continualization method

1 Introduction

Continualization methods may represent successful tools to identify and model the effects of the macroscopic behavior on the overall properties of MEE periodic materials. In the literature, there are continualization techniques that introduce the spatial discrete Fourier transform or the $\mathcal{Z}$-transform in the field equations involving Lagrangian systems, by achieving integral-differential equations of the equivalent non-local continuum with respect to the continuous displacement field. Then, the integral-differential equations may be approximated by higher order differential equations by considering the integral kernel as a Taylor series or as a Padé approximant, [1]. The current state-of-the art literature inspires the present work that proposes a dynamic multifield continualization approach for the analysis of MEE periodic materials and the study of coupled magneto-electro-elastic waves propagating through them. The field equations governing a MEE periodic heterogeneous material are provided. In particular, the case of a MEE layered material with a periodic microstructure is considered. The equations are analytically tackled by using complex auxiliary variables that allow halving the model dimension. The Floquet-Bloch theory and the transfer matrix method allow determining the linear parametric eigenproblem governing the MEE dispersive waves oscillating transversally and traveling along the material. Finally, a continualization technique, based on the introduction of the $\mathcal{Z}$-transform, is proposed to identify multi-field integral-type and multi-field generalized gradient-type non-local continua.

2 Methods and main results

According to the Floquet-Bloch theory, the continuity condition $\boldsymbol{y}_m^+ = \boldsymbol{y}_{m+1}^-$ between two adjacent layers m and $m+1$ of a MEE layered periodic material leads to

$$\boldsymbol{y}_N^+ = \boldsymbol{T}(\omega)\boldsymbol{y}_1^-, \tag{1}$$

where $\boldsymbol{T}(\omega) = \prod_{i=0}^{N-1} \boldsymbol{T}_{N-i}$ is the transfer matrix of the periodic cell, $\boldsymbol{y}_N^+$ is the generalized vector collecting the nodal displacement, the electric field, the magnetic induction field and the stress at the upper boundary of the last N-th layer and $\boldsymbol{y}_1^-$ is the generalized vector at the lower boundary of the first layer, [2]. The $\mathcal{Z}-$ transform of $\boldsymbol{y}$ in (1) is matched to the spacial Fourier transform with complex argument of the continuous field $\check{\boldsymbol{P}}(x_1, \omega)$, which leads to the integral-differential equation in the physical space and in the time domain. After some manipulations, the governing field equation of a multi-field generalized gradient-type non-local continuum with the integral-type inertial term is derived, [3]. The dispersion spectra are parametrically analysed for a two-layered periodic material as in Figure 1.

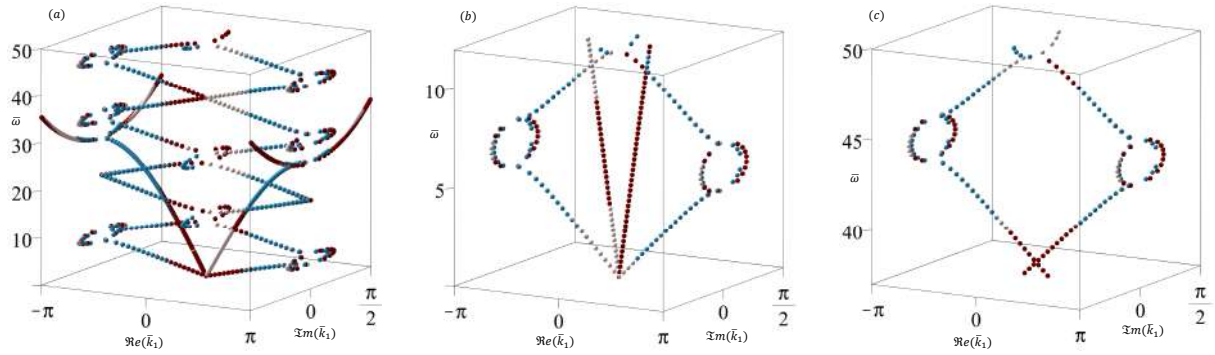


Figure 1: Comparison between the homogenized complex spectra (blue and white) and exact one (red) for different range of $\bar{\omega}$. In the zoomed views, stop-stop (b) and pass–stop (c) bands of frequencies are observed.

3 Conclusions

The propagation of electro-magneto-mechanics waves travelling along the direction perpendicular to a MEE material layering is investigated and a dynamic multifield continualization method has been outlined.

References

[1] Bacigalupo A, Gambarotta L. Identification of non-local continua for lattice-like materials. International Journal of Engineering Science 2021;159:103430.

[2] Del Toro R, Bacigalupo A, Lepidi M, Mazzino A. Dispersive waves in magneto-electro-elastic periodic waveguides. International Journal of Mechanical Sciences 2022; 236:107759.

[3] Del Toro R, De Bellis ML, Bacigalupo A. High frequency multifield continualization scheme for layered magneto-electro-elastic materials. Submitted 2023.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Image-based wave propagation analysis in large domains with irregular geometry using the SBFEM

S. Nattoji-Shara*, C. Birk* and H. Gravenkamp†

* Department of Civil Engineering
Institute of Structural Analysis, University of Duisburg-Essen
45141 Essen, Germany
e-mail: sharath.nattoji-shara@uni-due.de, carolin.birk@uni-due.de

† International Centre for Numerical Methods in Engineering
Universitat Politècnica de Catalunya
08034 Barcelona
e-mail: hgravenkamp@cimne.upc.edu

Abstract: The simulation of wave propagation phenomena (e.g., seismic waves) is numerically challenging, particularly due to the restrictions placed on the spatial as well as on the temporal discretization. For a large heterogeneous domain with several geometric irregularities, restrictions are imposed on meshing the considered domain; namely, a certain number of nodes per wavelength is required. The smallest distance between any two nodes in the discretized domain is one of the factors that determine the size of the time-step of the adopted transient solver. These rigorous requirements significantly increase the meshing burden and computational effort, whenever waves of high-frequency or short wavelength are of interest.

Efficient numerical tools, such as the finite element method (FEM) with spectral elements, are needed to simulate wave propagation phenomena. Due to the large size of the considered domain, a fast and robust technique is essential to discretize the domain. Image-based analysis using pixel/voxel-based domain discretization is one such approach that decomposes the domain into square/cube-shaped subdomains[1, 2]. The presence of hanging nodes, however, limits the application of FEM. The scaled boundary finite element method (SBFEM) can be employed to overcome the aforementioned limitation, where only the boundaries of subdomains are discretized. The SBFEM subdomains can be classified based on the position of the hanging nodes present on their boundaries. As a result, it is sufficient to compute the properties of one member of a pattern and later replicate it to its other members [1]. Moreover, high-order elements, which require fewer nodes per wavelength, can easily be incorporated into the SBFEM.

With the assumption of mass-proportional damping, a transient explicit solver typically involves the inversion of a mass matrix. The full potential of such a solver is realized by diagonalizing the mass matrix. Lumping the mass matrix entails matrix-vector multiplication, that efficiently computes the nodal displacements, thereby eliminating the need to solve a system of linear equations. If the subdomain boundaries are interpolated using linear or quadratic node-based shape functions, mass lumping can be achieved without loss of accuracy. For interpolation order > 2, no mass lumping scheme is known that guarantees optimal accuracy and positive definite mass matrices in the SBFEM [3].

For a specific application, it is not straightforward to predict whether the highest gain in efficiency is obtained by adopting an explicit time-stepping scheme, where the domain is discretized using low-order elements together with mass lumping, or by adopting an implicit time-stepping scheme in which tailored meshes of high-order elements are employed.

In this contribution, the results of the explicit time-stepping scheme, where the similarity of SBFEM elements are exploited, are compared with other time integration schemes. A couple of examples will be presented to illustrate the above aspects of time-domain simulation in heterogeneous domains.

Keywords: scaled boundary finite element method, Image-based analysis, Wave propagation, Mass lumping, Transient explicit solver

Acknowledgements

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - 418778046.

References

[1] A. Saputra, H. Talebi, D. Tran, C. Birk, C. Song, Automatic image-based stress analysis by the scaled boundary finite element method, *International Journal for Numerical Methods in Engineering*, vol.**109**, pp. 697–738, (2017).

[2] C. Birk and C. Song, Numerical modelling of seismic waves using image-processing and quadtree meshes, *Proceedings of 23rd Australasian Conference on the Mechanics of Structures and Materials (ACMSM23)*, vol. II, pp. 819–824, (2014).

[3] H. Gravenkamp, C. Song, J. Zhang, On mass lumping and explicit dynamics in the scaled boundary finite element method, *Computer Methods in Applied Mechanics and Engineering*, vol. **370** 113274, (2020).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Introduction of Octree meshes in regular prismatic structures using a combination of the Mortar Method and the Scaled Boundary Finite Element Method to simulate Ultrasonics Guided Waves

Lozano Daniel* **and Bulling Jannis†**

* 8.4 div. Acoustic and Electromagnetic Methods
Federal Institute for Materials Research and Testing (BAM)
Berlin, Germany
e-mail: daniel-hernando.lozano-duarte@bam.de

† 8.4 div. Acoustic and Electromagnetic Methods
Federal Institute for Materials Research and Testing (BAM)
Berlin, Germany
e-mail: jannis.bulling@bam.de

Abstract: Ultrasonic guided waves interacting with complex geometrical features are of high interest in the SHM field. For example, investigations into the extent to which a small change in defect geometry affects wave propagation have applications in Probability of Detection and defect reconstruction. These fields have to be supported by numerical tools aiming to retrieve accurate and reliable results and, thus, more realistic modeling. Due to the short wavelengths of ultrasonic waves and the relatively large domains in which the waves propagate, fine grid resolution for the entire domain is usually not possible due to limited computational resources. One solution is to partition the domain into different subdomains and use a specific, efficient approach for each subdomain. This contribution shows a combination of methods that aims to study these wave defect interactions in an elastic media. Firstly we introduce high-order 3D meshes that can resolve very fine geometrical details and are based on an Octree discretisation technique that employs special transition shape functions to resolve the hanging nodes that may appear due to the nature of the method. Afterward, the Octree mesh is embedded in a prismatic wave-guide based on the semi-analytical formulation of the SBFEM in 3D. To couple the different domains, we employ the mortar method, which enforces the continuity of the wave field across the internal boundaries of the domains. Examples show the power of the approach especially when it comes to parametric analysis.

Keywords: Elastodynamics, SBFEM, Octrees

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Comparison and validation of extended spectral element methods for structural health monitoring applications

Sergio Nicoli*, Konstantinos Agathos†, Pawel Kudela‡ and Eleni Chatzi*

* Department of Civil, Environmental, and Geomatic Engineering
ETH Zürich
Stefano-Franscini-Platz 5, CH-8093 Zürich, Switzerland
e-mail: {nicoli, chatzi}@ibk.baug.ethz.ch

† College of Engineering, Mathematics and Physical Science
Exeter University
Exeter, UK
e-mail: K.Agathos@exeter.ac.uk

‡ Institute of Fluid-Flow Machinery,
Polish Academy of Sciences,
Fiszera 14, 80-231 Gdańsk, Poland
e-mail: pk@imp.gda.pl

Abstract: In Structural Health Monitoring (SHM) with Guided Waves (GWs), data generated from sensor installations or sporadic inspections can be processed by simulating numerous damage scenarios of a structure, which are gradually updated as to match the recorded signal. This shows promising prospects of detecting, localizing, and even classifying small damage; however, it poses several challenges in terms of mechanical modeling and computational cost. In essence, the two main hurdles lie in the need for high resolution models, and in the limitations of traditional meshing software when automatically modeling localized features such as cracks and holes.

In addressing the first challenge, the Spectral Element Method (SEM) is selected as a basis for discretization, a choice which is motivated by its efficient high-order Ansatz space as well as by an optimally lumped mass matrix. Consequently, fast time-marching algorithms can be employed for solution of the equations of motion, without compromising the convergence properties of the model. Secondly, localized damage in the form of cracks can be introduced by extending Spectral Elements (SEs) via partition of unity enrichment functions, as in the eXtended Finite Element Method (XFEM).

In order to adopt these strategies in an explicit dynamics context, mass lumping methods for enriched SEs must be formulated. Importantly, optimal lumping of SEs is incompatible with the customized integration routines necessary in the presence of discontinuous enrichment functions. To overcome this, available mass lumping methods are sourced from the literature, and an alternative approach based on non-linear moment fitting is investigated. As a further alternative, the adoption of a hybrid implicit-explicit solver is also considered, which overcomes the need for the lumping of enriched elements at the price of a partially implicit solution.

Numerical examples involve cracked aluminum panels and plates, which enable to establish qualities and draw-backs of all the investigated approaches. Finally, this framework is applied in the modeling of a composite plate with multiple delamination-type damages and is validated by experimental measurements.

Keywords: SHM, Guided Waves, SEM, XFEM, Mass Lumping, Moment Fitting, Delamination

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Characterization of damage in steel plates by an inverse algorithm

Jannis Bulling*, Benjamin Jurgelucks†, Jens Prager* and Andrea Walther†

* Department of non-destructive testing
Bundesanstalt für Materialforschung und -pruefung (BAM), Unter den Eichen 87
12205 Berlin, Germany
e-mail: Jannis.Bullling@bam.de, Jens.Prager@bam.de

† Department of Mathematics
Humboldt-Universität zu Berlin, Unter den Linden 6
10099 Berlin, Germany
e-mail: Benjamin.Jurgelucks@math.hu-berlin.de, Andrea.Walther@math.hu-berlin.de

Abstract: The characterization of damage in shell-like structures, such as pipes, laminates, and plates, is particularly effective using ultrasonic guided waves by inspecting large areas of the structure starting from only a few sensor positions. However, damage sizing in particular is a challenging task in non-destructive testing and structural health monitoring, as the different dispersive modes of the guided waves do not always allow a simple correlation to be made between the reflections coming from the damage and the damage size. One way to determine the magnitude of the damage is to directly compare the measured signals with the signals from a simulation model. This reconstruction of the damage in the simulation model represents an inverse problem and an optimization problem. For the optimization, several forward calculations are needed to fit the damage model to the measured data.

Due to the short wavelengths of ultrasonic waves, classical methods for forward calculations, such as the finite element method (FEM), are often too computationally intensive. One way to reduce the computational cost is to approximate the wave propagation using the semi-analytical Scaled Boundary Finite Element Method (SBFEM). Previous studies have shown that the required degrees of freedom for the investigated domains and thus the computational time is much lower compared to the standard FEM.

In this contribution, a gradient-based optimization method for damage sizing is presented. The gradient of the SBFEM forward model is computed by Algorithmic Differentiation, allowing accurate and fast optimization. Examples include 2D cross-sectional models as well as 3D models of steel plates. The main focus will be on the numerical model and the properties of the inverse problem. The convergence of the proposed algorithm and its robustness to noise is presented. The validation of 2D models with experiments is briefly discussed.

Keywords: Inverse Problem, Scaled Boundary Finite Element Method (SBFEM), Algorithmic Differentiation (AD)

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Mesh-convergence and gradient-enhanced models in blast simulations of concrete structures

Sjard Mathis Rosenbusch*, Daniel Balzani† and Jörg F. Unger*

* Bundesanstalt für Materialforschung und -prüfung (BAM)
Division 7.7 Modelling and Simulation
Unter den Eichen 87, 12205 Berlin, Germany
e-mail: sjard-mathis.rosenbusch@bam.de, joerg.unger@bam.de

† Ruhr-Universität Bochum
Department of Civil and Environmental Engineering
Chair of Continuum Mechanics
P.O. Box No. 5, Universitätsstraße 150, 44801 Bochum, Germany
e-mail: daniel.balzani@rub.de

Abstract: Blast experiments on reinforced concrete structures are often limited to small structures and therefore simple shock waves. Such experiments are carried out at the Bundesanstalt für Materialforschung und -prüfung (BAM) and the structural response is investigated using several measuring methods. Complex load scenarios that occur as a result of reflection of the shock wave in larger structures are harder to realise in practice. Numerical simulations for the propagation of the shock wave and the structural response can therefore be an alternative method for the investigation of blast loads on complex structures.
For the simulation of concrete under impact and blast loads, several local constitutive models exist that are formulated as plasticity models with softening taken into account by introducing a scalar damage field. Local damage models however often lead to mesh-dependent results which do not converge with mesh refinement. In order to achieve meaningful predictions from numerical experiments, independence from the mesh is needed.
In this contribution, the JH2 model [3] with a parameter set for concrete is investigated in a simple blast load scenario. The shockwave is implemented as a simplified Friedlander-curve and the overpressures are applied as a boundary condition for the structural simulation. In order to account for large displacements that can occur during blast loads, an updated Lagrangian formulation is utilised. A Runge-Kutta method with adaptive time stepping is used to advance the solution in time. The open source FEM software FEniCS [1] is used together with an implementation of the JH2 model which has been developed at BAM. An extensive convergence analysis with both timestep- and mesh-refinement is carried out to show the mesh dependency. In order to make the results independent of the mesh, possible nonlocal versions of the JH2 model with gradient-enhancement are presented. Since many damage models for concrete share the damage mechanism of the JH2 model, the application of the regularisation methods to more complex material models, like the RHT model [2], is also discussed. Advantages of a gradient-enhanced formulation to simulate dynamic strength increase of concrete is discussed as well.

Keywords: concrete modelling, explicit dynamics, gradient-enhancement, mesh-convergence

References

[1] G. N. Wells et al A. Logg, K.-A. Mardal, "Automated Solution of Differential Equations by the Finite Element Method". Springer, 2012.

[2] T. Borrvall, W. Riedel "The RHT concrete model in LS-DYNA". Proceedings of the 8th European LS-DYNA users conference, Strasbourg, 2011.

[3] G. R. Johnson and T. J. Holmquist, "An improved computational constitutive model for brittle materials". AIP Conference Proceedings 309, 1994.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Bone fracture risk prediction *in silico*: digital twins in healthcare

Alessandra Aldieri [1,3], Chiara Garavelli [2,3], Antonino A. La Mattina [2,3], Marco Palanca [2], Marco Viceconti [2,3]

[1] PolitoBIOMed Lab, Department of Mechanical and Aerosapce Engineering – Politecnico di Torino, Italy
[2] Department of Industrial Engineering, Alma Mater Studiorum - University of Bologna, Italy;
[3] Medical Technology Lab, IRCCS Istituto Ortopedico Rizzoli, Bologna, Italy

Abstract: Bone fracture events are expected to increase more and more, but the current gold standards for assessing the patient-specific fracture risk have shown to have poor stratification accucray. Fractures cause a decreased quality of life and increased mortality, placing a significant social and economic burden. Therefore, improved prediction of the fracture risk would be crucial as it would foster preventive interventions before fracture occurs. In this context, a crucial role is being more and more played by patient-specific computational models used to inform the clinical decision, the so-called Digital Twins in Healthcare (DTH). Here we report the example of the Bologna Biomechanical Computed Tomography (BBCT)-hip and BBCT-spine, two patient-specific computational models at two different development stages to become DTH.

Keywords: Bone, fracture prediction, in silico, digital twin, ageing, FE

1. Introduction

Fragility fractures, which are very common both at the hip and at the spine, represent a more and more frequent evidence of an ageing society [1]. Ageing causes an overall bone loss and the deterioration of bone mechanical properties, which together result in a bone more prone to fractures. In parallel, as the treatment of cancer improves, the survival of patients affected by metastates increases. Metastates, which ofter interest the spine, alter the mechanical competence of the bone as well, increasing the susceptibility to fractures of already fragile subjects [2]. As a whole, bone fractures pose huge social and economic burdens: tertiary prevention is therefore crucial, and an accurate prediction of the actual risk of fracture would be crucial in preventing fracture through specific interventions. In this context, computational models able to provide insights currently not achievable otherwise and to outperform the gold-standards in the fracture prediction will come to play a major role in the future. In this work we present the *in silico* methodology Bologna Biomechaical Computer Tomography (BBCT)-hip and spine, developed for the fracture risk prediction at the femur and at the spine.

2. BBCT

BBCT-hip predicts the absolute risk of fracture (ARF0) for a subject based on his QCT images, height and weight. More in detail, a patient-specific Quantitative Computed Tomography (QCT)-based FE model predicts the load to failure, i.e. the load causing fracture, based on principal strains criteria. In parallel, an inverse pendulum analytical stochastic model calulates the impact forces due to a fall on the side. One million possible impact forces are computed and compared to corresponding one million loads to failure along possible femur poses at impact. ARF0 is calculated as the ratio of the impact forces exceeding the load to failure, i.e. causing fracture, to the total number of impact forces. The predictive accuracy of BBCT-hip FE models was assessed against *ex vivo* experiments

(RMSE<15%) [3], [4], while its stratification accuracy was assessed on a pair-matched retrospective cohort (AUC=0.87) [5].

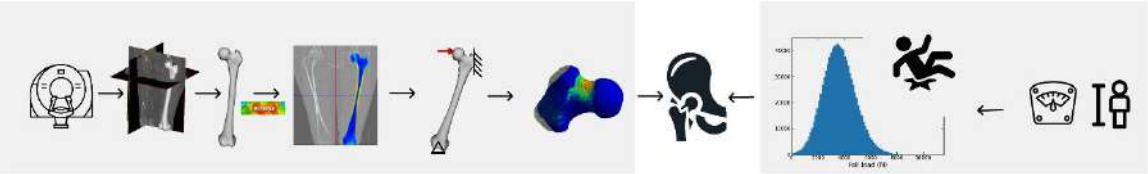


Figure 1. BBCT-hip workflow. On the left, the construction of the FE model to predict the load to failure, on the right, the impact force calculation model. Together, they allow to compute the absolute risk of fracture.

While clinical CT-based computational models for the fracture prediction at the femur have achieved a good level of maturity across the scientific community, much effort is currently being put on computational models of the spine. Here, a FE framework for spine segments is validated against *ex vivo* experimental data using Digital Image Correlation (DIC), a noncontact optical full-field measurement approach. Full-field displacements are primarily used for validation, representing the biomechanical variable primarily measured by DIC. Thoracolumbar four-vertebrae human spine segments were obtained from an ethically approved donation program. QCT images were acquired. Compression-flexion tests were performed loading each segment in elastic regime. A 4-camera state-of-art DIC (GOM Aramis 12M) was used to measure the displacement field on the vertebral body surfaces. FE models were generated from the QCT images using a 10-node tetrahedral mesh. Material properties of the bone were mapped elementwise [6], [7]. Intervertebral discs (IVDs) were modelled as linear elastic isotropic materials. The boundary conditions replicated the experimental test. FE-predicted displacements showed good agreement compared to DIC results in elastic regime (%RMSE <8%) [8], although the predicted deformations, on which the patient-specific fracture risk would be assessed, showed a significant degree of disagreement with respect to the experimental ones.

3. Conclusions

While mature existing DTH technologies (e.g. BBCT-hip) will have to be translated into use in specific clinical studies in order to provide scientific open-access evidence to health policymakers, experimental and computational studies will support the further development of DTH still at preliminary stage of development, such as BBCT-spine.

References

[1] J. A. Kanis, *et al.*, *Osteoporos. Int.*, vol. 30, fasc. 1, pp. 3–44, gen. 2019, doi: 10.1007/s00198-018-4704-5.
[2] S. Bailey, *et al.*, *J. Bone Miner. Res.*, vol. 37, fasc. 5, pp. 896–907, 2022, doi: 10.1002/jbmr.4539.
[3] E. Schileo, *et al.*, *J. Biomech.*, vol. 47, fasc. 14, pp. 3531–3538, nov. 2014, doi: 10.1016/j.jbiomech.2014.08.024.
[4] E. Schileo, *et al.*, *J. Biomech.*, vol. 40, fasc. 13, pp. 2982–2989, gen. 2007, doi: 10.1016/j.jbiomech.2007.02.010.
[5] A. Aldieri *et al.*, *Ann. Biomed. Eng.*, vol. 50, fasc. 3, pp. 303–313, mar. 2022, doi: 10.1007/s10439-022-02924-1.
[6] E. F. Morgan, *et al.*, *J. Biomech.*, vol. 36, fasc. 7, pp. 897–904, lug. 2003, doi: 10.1016/S0021-9290(03)00071-X.
[7] E. Schileo *et al.*, *J. Biomech.*, vol. 41, fasc. 11, pp. 2483–2491, ago. 2008, doi: 10.1016/j.jbiomech.2008.05.017.

[8] C. Garavelli, *et al.*, *PLOS ONE*, vol. 17, fasc. 9, p. e0272529, set. 2022, doi: 10.1371/journal.pone.0272529.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Experimental calibration of an in silico mechano-biological model of bone healing inflammatory response with the support of genetic algorithm.

Borgiani Edoardo[*,†], Nasello Gabriele[†] and Geris Liesbet[*,†]

[*] Biomechanics Research Unit
GIGA In Silico Medicine, University of Liège
Liège, Belgium

[†] Prometheus, division of Skeletal Tissue Engineering
Skeletal Biology and Engineering center, KU Leuven
Leuven, Belgium

Abstract: In recent years, *in silico* models have been promoted as valuable methods to investigate the mechano-biological hidden processes that support bone healing. We created a novel computer model that employs agent-based technique to investigate immune cells regulation during the inflammatory stage of bone healing. This model, combined with a mechano-regulated finite element model, will provide a new prospective on the investigation of mechano-biological aspects that supports early healing regulation. Immunofluorescent images are collected *in vivo* to calibrate the model. Quantitative comparison between the macrophage population counts in vivo and in silico allows a strict calibration of the model parameters. A genetic algorithm has been developed to iteratively adapt the parametric values to reduce the differences with the experimental results. After a few generations, the genetic algorithm found a combination of parameter values to calibrate the multiscale model. When those parameters are assigned to the model, the simulation output is characterized by minor quantitative differences with the experiments, contributing to a more realistic simulation result. Once the model will be fully calibrated and validated, it will provide a valuable support to the investigation of the hidden bone healing processes that are challenging to investigate experimentally.

Keywords: Bone fracture healing, computer model, inflammation, agent-based models, mechano-biology

1. INTRODUCTION

Bone fracture healing is a convoluted process that develops at multiple levels (tissue, cellular, molecular); therefore, using in silico multiscale modeling is highly appreciated to investigate its mechano-biological regulation. However, while numerous computer models have been developed to study the repair and remodeling phases of the process, only a few include also the initial inflammatory stage [1]. COMMBINI (COmputational Mechano-biological Model of Bone Injury Immunoresponse) aims to fill this gap as it will simulate mechanical and biological processes that occur within the bone fracture since the initial recruitment of inflammatory cells. We expect to obtain intriguing insights on novel treatments and therapeutics that might enhance the healing of the fracture from the first moments post-injury.

2. MATERIAL AND METHODS

COMMBINI uses an agent-based model [2] to reproduce biological events that happen at the molecular (pro- and anti-inflammatory cytokines) and cellular level (macrophages) in a 7 mm osteotomy performed in mice, iteratively simulated within a span of three days post-operation. The multiscale interactions are regulated by in vitro parametric values found in

the literature (e.g. [3]), which we propose to calibrate with in vivo immunofluorescent images [4]. The model is calibrated in two steps: sensitivity analysis, followed by evolutionary parametric optimization. Sensitivity analysis is performed on the in silico model parameters to evaluate the ones that primarily impact the quantitative outputs of the simulations. The evolutionary optimization employs a genetic algorithm (developed in-house with Python) to assess the combination of values that led the model outputs to a scenario more similar to the experimental one.

3. RESULTS

The model showed a strong sensitivity over the number of total macrophages to variations in the value of proliferation ratio, recruitment factor and debris engulfment. In particular, when optimization is performed over the proliferative parameter, the genetic algorithm converges to a lower ratio ($\hat{k}_p$= 5.34 10^{-4} min^{-1}) than the one found in literature (8.33 10^{-4} min^{-1} [3]) (Fig. 1).

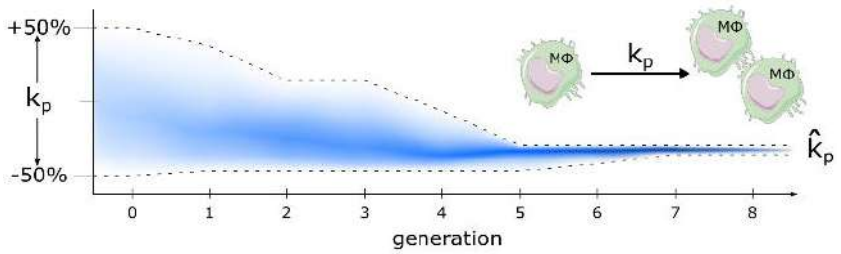


Figure 1. The genetic algorithm calibrates the model by converging to the optimal value for macrophage (MΦ) proliferation ratio ($\hat{k}_p$).

4. DISCUSSION AND CONCLUSIONS

COMMBINI is a novel multiscale in silico tool to explore the early stages of bone fracture healing. The agent-based model capacity to represent each single immune cell as a single entity allows the calibration with the support of experimental immunofluorescent images. Currently, the model is calibrated with quantitative in vivo data; however, it is planned to calibrate according to cell spatial distribution within the callus. Moreover, the coupling of COMMBINI with a mechanical model (finite element analysis, in development) will expand the investigation to mechano-regulated aspects during the inflammatory stage of bone healing.

References

[1] Lafuente-Gracia L, Borgiani E, Nasello G, Geris L. Towards in silico Models of the Inflammatory Response in Bone Fracture Healing. Front Bioeng Biotechnol. 2021;9:703725.

[2] Ghaffarizadeh A, Heiland R, Friedman SH, Mumenthaler SM, Macklin P. PhysiCell: An open source physics-based cell simulator for 3-D multicellular systems. PLoS Comput Biol. 2018;14(2):e1005991.

[3] Chitu V, Yeung YG, Yu W, Nandi S, Stanley ER. Measurement of macrophage growth and differentiation. Curr Protoc Immunol. 2011;Chapter 14:Unit-14.20.26.

[4] Schlundt C, El Khassawna T, Serra A, et al. Macrophages in bone fracture healing: Their essential role in endochondral ossification. Bone. 2018;106:78-89.

An innovative computational workflow for the design of self-expanding femoral artery stents using topology optimization

Carbonaro Dario, Politecnico di Torino, Turin, Italy, dario.carbonaro@polito.it

Mezzadri Francesco, Università degli studi di Modena e Reggio Emilia, Modena, Italy, fmezzadri@unimore.it

Perotto Simona, Politecnico di Milano, Milan, Italy, simona.perotto@polimi.it

Ferro Nicola, Politecnico di Milano, Milan, Italy, nicola.ferro@polimi.it

De Nisco Giuseppe, Politecnico di Torino, Turin, Italy, giuseppe.denisco@polito.it

Gallo Diego, Politecnico di Torino, Turin, Italy, diego.gallo@polito.it

Chiastra Claudio, Politecnico di Torino, Turin, Italy, claudio.chiastra@polito.it

Audenino Alberto, Politecnico di Torino, Turin, Italy, alberto. audenino@polito.it

Morbiducci Umberto, Politecnico di Torino, Turin, Italy, umberto.morbiducci@polito.it

Abstract: In this study, a computational framework was developed for the systematic design of next generation self-expandable femoral stents. Technically, stents were considered as made by a repeating unit cell, designed by combining topology optimization and inverse homogenization, so that the macroscopic stent structures satisfy prescribed design requirements. Five stent designs with different geometrical features were generated as a proof-of-concept. Finally, *in silico* tests were conducted to characterize the mechanical performance of the stents.

Keywords: femoral stent, topology optimization, finite element method, computational fluid dynamics.

1. Introduction

In-stent restenosis (ISR) is a major drawback that still limits the safety and success of femoral stenting. This complication is related to the stent geometry and to the mechanical interaction between the device and the vessel wall [1]. Accordingly, significant research efforts have been conducted to improve the stent design and several computational frameworks were developed to optimize the biomechanical performance of the devices. Nevertheless, the current development of femoral stents is still incremental, resulting in minimum modifications of the geometry as compared to the devices already available. Within this context, we present a computational workflow for the design of next generation self-expandable femoral artery stents. The proposed workflow employs inverse homogenization topology optimization (TO) to generate innovative 2D unit cells of the stent [2], which are then converted in 3D stent geometries and verified from both a structural and hemodynamic viewpoint.

2. Methods

The procedure for the design of self-expanding femoral artery stents consists of four main steps (Fig. 1). The inverse homogenization TO, that allows to design microstructures with prescribed properties at the macroscale, was adopted to generate 2D geometries of a single stent cell (Fig. 1A), with the aim of reducing the contact area between the stent and the arterial wall, and of controlling the radial stiffness and the foreshortening of the design. With this aim, we have exploited the microSIMPATY algorithm [2], which enriches a standard SIMP-based inverse homogenization TO process with the selection of a strategic (i.e., an anisotropic adapted) computational mesh. 3D stent geometries were obtained by scaling and repeating the 2D unit cells (Fig. 1B), which were thereafter projected to a cylinder and extruded to assign a constant strut thickness. Nonlinear structural finite element (FE) analyses of a complete crimping cycle were then conducted to characterize the mechanical performance of the stent designs (Fig. 1C). The

following three FE outputs were accounted to evaluate the mechanical performance of each design: the peak maximum principal strain of the stent, as a measure of device integrity throughout implantation procedure; the radial force magnitude as a measure of the radial stiffness of the device; the stent foreshortening, as a measure for the precise device placement into the vessel [3]. Thereafter, transient, laminar computational fluid dynamics (CFD) simulations were performed considering an idealized cylindrical femoral artery (Fig. 1D). The impact of the stent design on the hemodynamics and the associated risk for ISR was analysed in terms of time average wall shear stress (TAWSS) and topological shear variation index (TSVI) [4].

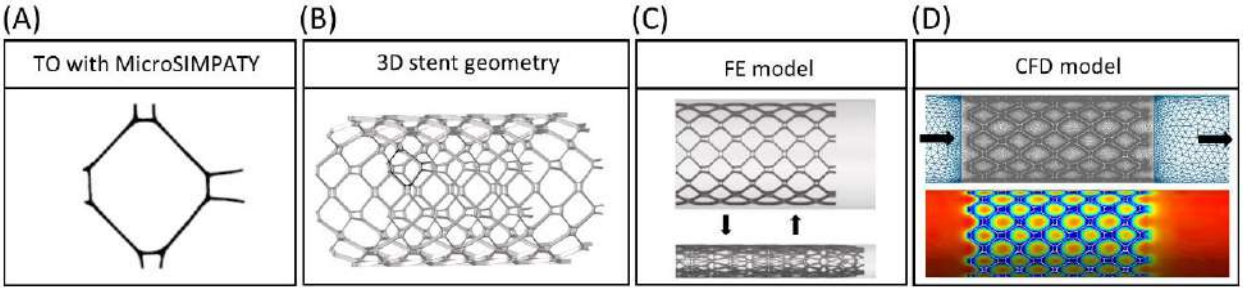


Figure 1. Main steps of the workflow for the design and verification of femoral artery stents.

3 Results and conclusion

Five proof-of-concept stent designs with different geometrical features (Fig. 2) were generated in the first step of the workflow (Fig. 1A). FE analyses indicated that only two stent designs (Fig. 2, designs 1 and 5) met the minimum requirement for usability throughout the implantation procedure. Moreover, it emerged that design 1 was better in terms of mechanical characteristics, while design 5 was better in terms of geometrical (i.e., lower contact area) and hemodynamic characteristics.

The developed computational framework allows to systematically obtain new designs of femoral artery stents, contributing to the reduction of time and costs associated with the *in vitro* bench testing campaign and conventional trial-and-error design methods.

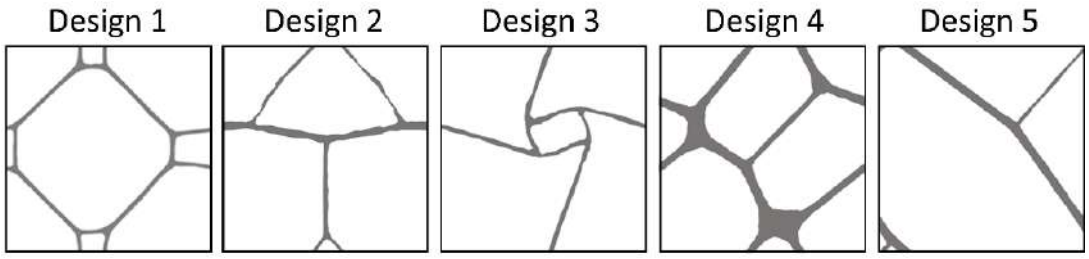


Figure 2. Five femoral stent designs generated with the proposed workflow.

References

[1] Shlofmitz E, et al., Circ Cardiovasc Interv 2019; 12: 1–8.

[2] Ferro N, et al., Lect Notes Comput Sci Eng, Springer Cham 2020; 132: 211-221.

[3] ISO, Cardiovascular implants - Endovascular devices - Part 2: Vascular stents 2010.

[4] Chiastra C, et al., J Biomech Eng 2022; 144: 061002.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Multiphysics Modelling of Vasodilation in Arteries

Bastien Sauty*, Claire Morin*, Stéphane Avril* and Michele Marino†

* Mines Saint-Etienne, Univ Jean Monnet Saint-Etienne, INSERM, U 1059 Sainbiose
Saint-Etienne, France
e-mail: bastien.sauty@emse.fr

† Department of Civil Engineering and Computer Science, University of Rome "Tor Vergata"
Rome, Italy

Abstract: Understanding the development of cardiovascular disease relies on the exploration of the interactions between the chemo-bio-mechanical behaviour of the local arterial tissues and the hemodynamics of the global cardiovascular system. The present work aims to introduce a new framework for modelling these multiphysics and multiscale processes in a coupled approach. In this study, the biochemical pathways responsible for vasodilation are explored in a model coupling a local multiphysics Finite Element model of the arterial tissue, and a global lumped 0D model of the cardiovascular system. As a bridge between multiphysics phenomona at different geometrical and temporal scales, this framework is a first step in the comprehensive approach exploring the interactions in the cardiovascular system leading to the development of pathologies.

Keywords: Vasodilation, Arterial Tissue, Multiphysics, Coupled 0D-3D models

1 Multiphysics and multiscales in arterial tissues

The physiological behaviour of the cardiovascular system is driven by the mechanical response of the arterial segments. Composed of both a passive elastic response of the extracellular matrix and an active reaction of the smooth muscle cells, it is therefore dependant on the tissue histological architecture and on the local biochemical state driving vasoconstriction. Furthermore, the cardiovascular system undergoes a continuous adaptation to the evolution of the blood flow, with a fast reversible response through the contractile tone of smooth muscle cells, and a slow response through growth and remodelling of the tissue. Cardiovascular diseases develop when remodelling is dysfunctional.

Hence, the study of cardiovascular diseases, such as chronic hypertension, relies on a comprehensive approach of the multiphysics problem, at the crossroad between mechanics, biology and chemical behaviour, but also on a multiscale description, both geometric and temporal, of these phenomena. Indeed, the global hemodynamic conditions of the cardiac cycle and the vasculatur resistance affect the local flow and in turn the internal tissue stresses driving biochemical signals. And, whereas the hemodynamic is evolving in seconds, biochemical processes have a characteristic time of minutes for the vasodilation and days for growth and remodelling.

To the best of the authors' knowledge, current litterature lacks a mathematical description of the arterial tissue that couples a lumped description of the cardiovascular system and a detailed continuum model of the local chemo-mechano-biological behaviour of the arterial

tissue for specific regions of interest. This work contributes to the development of comprehensive models able to explore the interactions leading to the development of cardiovascular pathologies.

2 Case study : Chemically driven Vasodilation

Vasodilation consists of the extension of smooth muscle cells to adapt the artery to an unbalanced blood flow, in order to maintain a preferred mechanical state in the arterial tissue (circumferential stresses and wall shear stresses) [1].

The framework consists in modelling the global scale of the cardiovascular system with a 0D lumped model and the local scale of the arterial tissue with a FEM of an arterial cross-section. Endothelial cells, under blood flow associated shear-stress, emit vasodilator species (Nitric Oxyde and Reactive Oxygen Species) affecting the vasotone of the Smooth Muscle Cells. The latters, within the Extra-Cellular Matrix, contract or dilate, changing both the geometry and compliance of the arterial section.

The model is tested with a short term increase of the blood flow, and results show that vasodilation limits the variation of shear stresses sensed by endothelial cells through an increase of the radius of the artery. Furthermore, vasodilation relaxes stresses in the extracellular matrix, which increases the compliance of the tissue, and therefore reduces the variation of pressure during a cardiac cycle. The numerical results are consistent with available experimental data.

3 Conclusions

This framework, as a versatile tool coupling simple but extendable models, is a basis for the modelling of cardiovascular diseases with the introduction of dysfunctional growth and remodelling of the arterial tissue. It is a first step into the building of hypothesis driven models exploring the etiology of cardiovascular diseases.

References

[1] Wilstein, Z., Mathematical Biosciences (2018), https://doi.org/10.1016/j.mbs.2018.05.002

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

An electromechanical heart-torso coupled model for the simulation of the ECG

Zappon Elena*, Salvador Matteo*, Piersanti Roberto*, Regazzoni Francesco*, Manzoni Andrea*, Dede' Luca*, and Quarteroni Alfio*,†

* MOX-Dipartimento di Matematica,
Politecnico di Milano,
Milano, Italy,
e-mail: elena.zappon@polimi.it, matteo.salvador@polimi.it, roberto.piersanti@polimi.it, francesco.regazzoni@polimi.it, andrea1.manzoni@polimi.it, luca.dede@polimi.it, alfio.quarteroni@polimi.it

† Institute of Mathematics,
Ecole Polytechnique Federale de Lausanne,
Lausanne, Switzerland (Professor Emeritus)

Abstract: The electrocardiogram (ECG) is the most widely used non-invasive diagnostic tool to gain insight into the electrical activity of the heart. Mathematically, it is usually simulated by a coupled multi-scale and multi-physics non-linear dynamical problem, called heart-torso model, describing the cardiac electrophysiology, however neglecting the effect of the underline myocardial mechanics. In this work, we present a novel electromechanical in-silico heart-torso (EMT) model, coupling a 3D-0D closed-loop electromechanical model for the heart, with a Laplace equation to represent the propagation of the cardiac electrical signal through the torso, moreover including the cardiac and torso deformations due to the myocardial contraction. Numerical simulations with the EMT model on a realistic in-silico biventricular geometry are performed, and the corresponding ECGs are compared with respect to the heart-torso model, both in sinus rhythm and under ventricular tachycardia.

Keywords: Electrocardiogram, Cardiac electromechanics, Cardiac electrophysiology, Heart-torso model.

1 Introduction

The ECG is the most widely used non-invasive diagnostic tool in cardiac electrophysiology (EP) [1]. A mathematical model able to reproduce the ECG is a coupled multi-scale and multi-physics problem, defined by a ODE-PDE non-linear system to simulate the cardiac EP, and a Laplace problem to compute the cardiac EP signal propagation in the human torso [2]. The solution of such model is carried out on 3D *static* domains, that of the heart and of the torso. However, the heart undergoes large deformations due to the myocardial contraction, that affect the propagation of the EP signal and, therefore, the ECG [3]. In this work we aim at accounting for such deformations proposing a new 3D-0D closed-loop electromechanical heart-torso model, coupling an electromechanical model for the heart [4], with the Laplace model in the torso [2], automatically shaping the torso domain according to the cardiac displacement. The model is then investigated on realistic geometries, both in sinus rhythm and under ventricular tachycardia.

2 Mathematical model

The EMT model is a multi-physics and multi-scaled model obtained coupling different mathematical models, able to comprehensively represent the major physical electromechanical

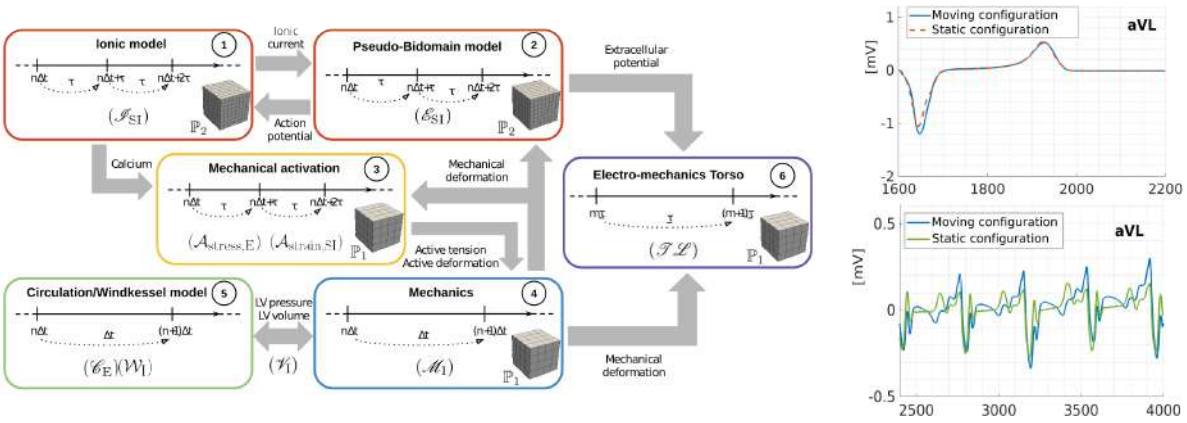


Figure 1: Numerical scheme of the EMT model (left), and example of ECG lead in sinus rhythm (top-right) and under ventricular tachycardia (bottom-right) considering either the heart-torso or the EMT models.

phenomena in the heart and in the human torso. Specifically, we employ the 3D-0D closed-loop cardiac electromechanical model presented in [4], which is able to describe the cardiac electrical activation, the active contraction at the sarcomeres level, the myocardial contraction, and the blood circulation. The passive mechanics in the human body is then simulated employing a lifting extension of the cardiac displacement on the torso. Finally, a Laplace equation is implemented in the torso domain, incorporating the displacement extension to mimic the cardiac deformation. A suitable segregated-intergrid-staggered numerical scheme (see Fig. 1) is then implemented to handle the different space-time scales required by the models involved [4], ensuring spatial and temporal flexibility.

3 Conclusions

The numerical tests are carried out on a realistic 3D in-silico biventricular geometry and on a realistic torso. Both healthy and pathological conditions, *e.g.* ventricular tachycardia, are simulated considering either static of moving domains. Fairness of the comparison is ensured by prescribing the same numerical and parameters setting in all simulations. The ECGs obtained for each simulations are then compared (see Fig. 1), showing that the effect of myocardial contraction on the electric signal propagation withing the body, and thus on the ECG, cannot be neglected, especially in pathological conditions.

References

[1] S. Monaci, al. In-silico pace-mapping using a detailed whole torso model and implanted electronic device electrograms for more efficient ablation planning. Computers in Biology and Medicine, 2020.

[2] P. Colli Franzone, et al. Mathematical Cardiac Electrophysiology. Springer MS&A Series, Vol. 13, 2014.

[3] R. Andlauer, et al. Influence of left atrial size on P-wave morphology: differential effects of dilation and hypertrophy. EP Europace, Vol. 20, 2018.

[4] R. Piersanti, et al, 3D–0D closed-loop model for the simulation of cardiac biventricular electromechanics, Computer Methods in Applied Mechanics and Engineering, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Phase-field modeling of brittle fracture in heterogeneous bars

Vicentini Francesco*, Carrara Pietro* and De Lorenzis Laura*

* Department of Mechanical and Process Engineering (D-MAVT)
ETH Zürich
Zurich, Switzerland
e-mail: fvicentini@ethz.ch

Abstract: Through phase-field modeling of brittle fracture, we investigate how the continuous variation of elastic modulus and/or fracture toughness along a 1D bar affects key observed quantities, such as the peak stress and the dissipated energy upon fracture, and, consequently, the location of the predicted crack. Thus, it is shown that the effect of heterogeneity is strictly related to the non-local nature of the phase-field model.

Keywords: Heterogeneity, Phase-field, 1D, Fracture toughness, Peak stress

1 Introduction

Phase-field modeling of brittle fracture [1] is particularly attractive for heterogeneous materials, such as bone, due to its ability to predict nucleation and propagation of cracks with arbitrarily complex patterns with no need for ad hoc criteria. Previous studies addressing fracture in heterogenous materials have adopted a pragmatic approach and are exclusively numerical. A fundamental mathematical analysis of the key phase-field predictions is available only for the assumption of homogeneous material [1]. In our contribution, we perform such missing investigation for the one-dimensional case by assuming continuous variation of the elastic and/or fracture properties. Our main goal is to quantitatively assess how the heterogeneity in material properties influences the peak stress and the dissipated energy upon fracture.

2 Model

The analysed 1D bar is defined over the interval $(-L, L)$, clamped on one end and pulled on the other through displacement control. Using the `AT1` formulation, the phase-field approach consists in the minimization of the energy functional

$$\mathcal{E}(u,\alpha) = \underbrace{\int_{-L}^{L} \frac{1}{2}\,(1-\alpha)^2\,E_0\,u^2\,dx}_{\text{elastic energy}} + \underbrace{\frac{3}{8}\int_{-L}^{L} G_c(x)\,\left(\frac{\alpha}{\ell}+\ell\,\alpha'^2\right)\,dx}_{\text{dissipation}} \quad \text{with} \quad G_c(x) = \bar{G}_c\left(1+\frac{|x|}{\ell_w}\right), \qquad (1)$$

where u is the displacement and $\alpha \in [0,1]$ the local damage ($\alpha = 0$: sound material, $\alpha = 1$: fully broken material). The non-locality of the model requires the introduction of an internal length ℓ that controls the size of the support of α upon localization. We have assumed here that the elastic modulus E_0 is constant along x, whereas the fracture toughness features a V-shape distribution $G_c(x)$ with a minimum at $x = 0$. The length ℓ_w is the reciprocal of the V slope and its associated dimensionless group is the characteristic ratio $r = \ell/\ell_w$. The limit operation $r \to 0$ returns a *reference* homogeneous material.

3 Conclusions

By solving analytically or semi-analytically the Karush-Kuhn-Tucker conditions stemming from Eq. 1, we draw the following conclusions:

- The elastic limit stress for the heterogeneous bar is the same as for the bar made of the reference homogeneous material;
- The evolution problem for the heterogeneous bar does not admit a homogeneous solution in the damaging phase;
- The peak stress $\sigma_p = \bar{\sigma}_p\, s(r)$, where $\bar{\sigma}_p$ is the peak stress for the reference homogeneous material and $s(r)$ is a monotonically increasing function of r with $s(0) = 1.$;
- The dissipated energy at crack onset $D_u = \bar{D}_u\, g(r)$, where $\bar{D}_u$ is the dissipated energy for the reference homogeneous material and $g(r)$ is a monotonically increasing function of r with $g(0) = 1$.

The observed effects of heterogeneity are consequences of the non-local nature of the phase-field model. This becomes evident when considering mutliple minima competing as location of crack onset (see as example Fig. 1).

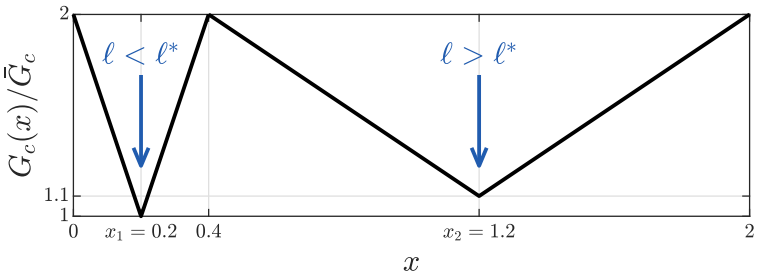


Figure 1: Example of a 2-length bar in tension with heterogeneity in G_c. The crack location (blue arrow) depends on the length-scale parameter: the crack forms at x_1 if $\ell < \ell^*$ and at x_2 if $\ell > \ell^*$, with $\ell^* \simeq 0.056$.

These results are also valid for different shapes of heterogeneity and for heterogeneity in E_0 and can be extended to a bar embedded in the three-dimensional space [2].

References

[1] Pham K, Amor H, Marigo JJ, Maurini C. Gradient damage models and their use to approximate brittle fracture. International Journal of Damage Mechanics. 2011 May;20(4):618-52.

[2] Vicentini F, Carrara P, De Lorenzis L. Phase-field modeling of brittle fracture in heterogeneous bars. European Journal of Mechanics-A/Solids. 2023 Jan 1;97:104826.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A microstructure-informed model of the white matter of human brain

Michele Terzano[1], Saeideh Saeidi[1], Manuel P. Kainz[1], Misael Dalbosco[1,2] and Gerhard A. Holzapfel[1,3]

[1] Institute of Biomechanics
Graz University of Technology, Graz, Austria
e-mail: michele.terzano@tugraz.at

[2] GRANTE – Department of Mechanical Engineering
Federal University of Santa Catarina, Florianópolis, SC, Brazil

[3] Department of Structural Engineering
Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Abstract: We propose a micromechanical model of the brain white matter, which is described as a heterogeneous tissue with axonal fibers embedded in a soft substance that forms the ground matrix. Our approach is developed within the framework of continuum microstructure-based models of reinforced composites. The microscale is described by a representative volume element (RVE), reinforced with embedded fibers and implemented in the finite element method to derive the homogenized macroscale response. The behavior of each constituent is described by a nonlinear isotropic viscoelastic material model. Microscale features such as axon fiber orientation, distribution of axon diameters, and tortuosity are directly included from experimental observations. The model is validated by simulating elementary deformations and comparing the homogenized response with existing experimental data. Furthermore, a sensitivity study is performed to show the influence of mechanical and microstructural model parameters on the tissue-scale response. The proposed computational model can improve the accuracy of biomechanical simulations of the human brain in both healthy and pathological states by establishing a direct relationship between macroscopic behavior and underlying microstructural features.

Keywords: brain; microscale; fibers; representative volume element; finite element method

1. Introduction

The brain is one of the most important and complex organs in the human body. Its structure is highly heterogeneous, with fairly dense gray matter regions containing mainly neuronal cell bodies and fibrous white matter regions characterized by axons, astrocytes and microglial cells [1]. The mechanical behavior of the human brain is typical of a supersoft, highly nonlinear material with remarkable time-dependence. To date, a variety of isotropic and anisotropic constitutive models have been proposed to characterize the nonlinear macroscale response of the tissue under arbitrary loading conditions. However, when these models are developed on purely phenomenological formulations, they lack a physical connection to the underlying microstructural composition and often require a large number of fitted parameters.

As an alternative, we propose here a continuum micromechanical model, in which the microstructure of the tissue is explicitely considered in the formulation. Based on an RVE, the homogenized response of the tissue is derived numerically within the finite element (FE) method [2]. The approach proposed is applied to the human brain white matter, here schematized as a continuum with embedded axonal fibers, and validated through a comparison with experimental data [3]. The aim of this work is to demonstrate the correlation between microstructural features accessible by direct observation and the mechanical response at the tissue level. This can improve our understanding of the biomechanics of the healthy human brain and provide insight into the variations that occur with aging or neurodegeneration.

2. Methods

White matter RVEs are modeled as cubes with three-dimensional continuum elements, representing the ground matrix, and uniaxial truss embedded elements for the axonal fibers. Axons are randomly distributed within the RVE without intersection, considering a specific volume fraction and orientation according to histological images, in addition to a distribution of axon diameters acquired from electron microscopy. The tissue constituents are modeled as isotropic finite strain viscoelastic materials. In addition, the constitutive law of axonal fibers is modified to include the tortuosity obtained from experimental observations [4] through the concept of recruitment stretch. A no-compression behavior is specified to account for the fiber buckling. Linear boundary displacements are applied to ensure deformation compatibility and the periodic behavior of the RVE. The macroscale response is captured by the homogenized stress [3].

The FE model is applied to simulate a set of selected elementary loading cases of tension along and transverse to the axons and simple shear. First, the mechanical and structural parameters are tuned to reproduce experimental results on human corpus callosum and to validate the approach proposed. A sensitivity study is then carried out to show the influence of the different parameters. All analyses are performed with the commercial software Abaqus using custom Python scripts and a user material subroutine.

3. Results

Preliminary analyses were performed to test the convergence of the macroscopic response with respect to the size of the RVE. We considered four different cube sizes with side lengths ranging from 5 to 50 micrometers and approximately 24 to 2900 axonal fibers. As expected, the response shows a convergence-like trend with increasing size and the homogenized stress (median) is well within the bounds of the experimental data.

4. Conclusions

The proposed model is able to capture several microstructural features that characterize the mechanical behavior of human white matter. Simulations of experimental tension along and tranverse to the axonal fibers indicate an influence of structural anisotropy on the mechanical response of the human brain, at least for this highly oriented white matter region. The numerical implementation in commercial finite element software makes our approach very attractive for large-scale simulation of brain biomechanics.

References

[1] Budday S, Ovaert TC, Holzapfel GA, Steinmann P, Kuhl E. Fifty shades of brain: a review on the mechanical testing and modeling of brain tissue. Arch Comput Methods Eng 2020; 27:1187–1230.
[2] Dalbosco M, Carniel TA, Fancello EA, Holzapfel GA. Multiscale numerical analyses of arterial tissue with embedded elements in the finite strain regime. Comput Methods Appl Mech Eng 2021; 381:113844.
[3] Budday S, Sommer G, Birkl C, Langkammer C, Haybaeck J, Kohnert J, Bauer M, Paulsen F, Steinmann P, Kuhl E, Holzapfel GA. Mechanical characterization of human brain tissue. Acta Biomater 2017; 48:319–340.
[4] Bernardini A, Trovatelli M, Kłosowski MM, Pederzani M, Zani DD, Brizzola S, Porter A, Rodriguez y Baena F, Dini D. Reconstruction of ovine axonal cytoarchitecture enables more accurate models of brain biomechanics. Commun Biol 2022; 5:1101.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Process design in extrusion-based bioprinting

Chirianni Francesco*, Vairo Giuseppe* and Marino Michele*

* Department of Civil Engineering and Computer Science (DICII)
University of Rome Tor Vergata
Rome, Italy
e-mail: chirianni@ing.uniroma2.it, vairo@ing.uniroma2.it, m.marino@ing.uniroma2.it

Abstract: Extrusion-based bioprinting is an additive manufacturing technique able to produce engineered tissues through layer-by-layer deposition of viable cells suspended in a biomaterial solution. The printing mechanism can expose cells to damage induced by stresses that arise during the extrusion process. The resulting cell damage can severely affect the function of the printed constructs. In order to ensure an acceptable level of cell damage, specific process variables (e.g., geometry of the extruder and dispensing pressure) must be properly chosen. Unfortunately, the relationship between bioprinting process variables and the effectiveness of the final printed structure (e.g., in terms of resolution and cell viability) is governed by complex and nonlinear mechanisms. Hence, the optimal setting of the printing workflow in laboratory practice is generally obtained from an expensive and time-consuming trial-and-error procedure. The aim of this work is to speed-up the definition of optimal printing conditions, thus reducing the cost for their definition, by summarizing the interrelations between fundamental process variables with a reduced-order model developed from few detailed numerical simulations. Through this reduced-order model nomograms are built to provide laboratories with fast graphical calculations that synthesize the complex relationship between coupled process variables.

Keywords: Extrusion-based bioprinting, Non-Newtonian fluids, FEM, Reduced-order model, Nomograms.

1 Introduction

Extrusion-based bioprinting is an additive manufacturing technique able to produce engineered tissues through layer-by-layer deposition of a bio-ink (viable cells suspended in a biomaterial solution) [1]. The extrudability of a bio-ink and the corresponding printing settings are determined by the rheological behaviour, generally shear-thinning.

The printing mechanism can expose cells to damage induced by shear and extensional stresses that arise during the extrusion process [2,3]. The resulting cell damage can severely reduce cell viability and affect the function of the printed constructs. In order to maintain stresses below a threshold value that ensures an acceptable level of cell damage, specific process variables such as diameter of the needle and dispensing pressure must be properly chosen. Unfortunately, due to the interplay of mechanical and biological phenomena, the relationship between bioprinting process variables and the effectiveness of the final bioprinted structure (e.g., in terms of resolution and cell viability) is governed by complex and nonlinear mechanisms. Hence, the optimal setting of the printing workflow in laboratory practice is generally obtained from an expensive trial-and-error procedure.

The aim of this work is to speed-up the definition of optimal printing conditions, thus reducing the cost for their definition, by summarizing the interrelations between fundamental

process variables through the construction of nomograms.

2 Methods

The approach pursued to simulate the extrusion process is based on the numerical solution of a fluid-dynamics problem where the bio-ink is modelled as an incompressible viscous non-Newtonian fluid with shear-thinning flow behaviour. Numerical simulations have been performed using the finite element method (FEM) with mixed Galerkin formulation. An appropriate axisymmetric P2P1 triangular element has been implemented.

Numerical results have been employed, together with theoretical considerations, to define a reduced-order model able to describe the mutual correlation among fundamental process variables. Through these semi-analytical relationships nomograms are built. For the construction of cell damage isopleths a cell damage law has been introduced on the basis of experimental data reported in [3].

3 Conclusions

A nomogram, see Figure 1, has been built from the developed reduced-order model. Isopleths allow to quickly estimate cell damage under different printing conditions.

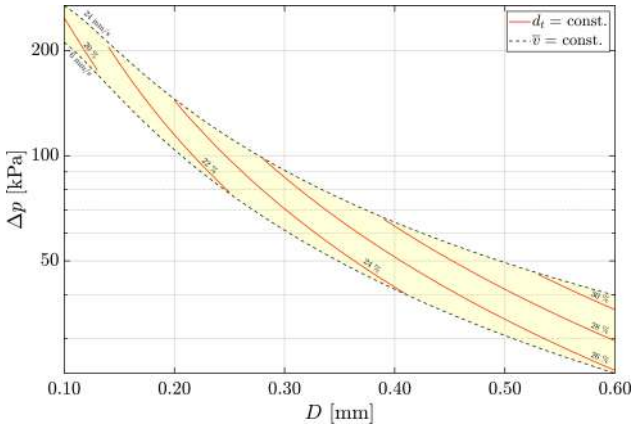


Figure 1: Nomogram with iso-damage curves built from the developed reduced-order model.

References

[1] Ozbolat IT, Hospodiuk M. Current advances and future perspectives in extrusion-based bioprinting. Biomaterials 2016;76:321-343.

[2] Ning L, Betancourt N, Schreyer DJ, Chen X. Characterization of cell damage and proliferative ability during and after bioprinting. ACS Biomater Sci Eng 2018;4:3906-3918.

[3] Han S, Kim CM, Jin S, KIm TY. Study of the process-induced cell damage in forced extrusion bioprinting. Biofabrication 2021;13:035048.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Constitutive modelling of hydrogels for tissue-developing bio-printing applications

Zoboli Lorenzo*, Gaziano Pierfrancesco†, Gizzi Alessio*, Vairo Giuseppe†, and Marino Michele†

* Nonlinear Physics and Mathematical Modelling Laboratory
Campus Bio-Medico University of Rome
Rome, Italy
e-mail: lorenzo.zoboli@unicampus.it

† Department of Civil Engineering and Computer Science (DICII)
Univeristy of Rome Tor Vergata
Rome, Italy

Abstract: The objective of modern bio-printing techniques is to reproduce the desired target tissue by extruding a gel containing stem cells into a determined pattern and immersing it in a specific culture environment. The cells will feed on the culture nutrients and grow into a specialised tissue array. The applications of this concept are almost boundless, from patient-specific prosthetics to cultivated meat production, but particular care must be devoted to the characterisation and control of the stages following the printing process itself. This work illustrates an advanced modelling strategy of the photon-assisted transformation of the bio-ink containing the cells into a structured polymer gel, a process occurring shortly after the ejection form the extruder. The modelling strategy is based on a Finite Element formulation that accounts for light-activated chemical kinetics, non-linear deformations and heat diffusion.

Keywords: Bioprinting, polymer modelling, FEM, multi-coupled problems

1 Introduction

The background of this research is the controlled production of cultivated meat, which is possible today drawing on the capability for stem cells to reproduce various type of cells, including muscle or fat ones [1]. To grow a selected type of tissue, stem cells must firstly be contained into a hosting structure (*construct*) and then they must be fed specific nutrients to trigger cellular differentiation. In this respect, 3D printing is an ideal technique because it extrudes a semi-viscous material (printing ink, which in this case is called a *bio-ink*) that rapidly solidifies (in this case it *gels*) and is ready for successive manipulation. The basic idea behind cultivated meat is therefore to build a bio-ink by embedding stem cells into an hydrogel, print it into a layered construct, and feed it nutrients. After its deposition, the bio-ink is immersed into $CaCl_2$ and UV light is irradiated onto it. This activates polymerisation reactions that merge together individual monomers contained in the hydrogel to form polymer chains, and ultimately brings the newly printed matrix from a viscous melt state to a gel state. Cross-linking of partial polymer chains into a network of longer polymer chains is directly related to the viscosity and stiffness of the gelified bio-ink. Control of this process is of pivotal importance, since cellular motility and nutrient diffusion are greatly affected by the disposition and orientation of this polymer network.

2 State-of-the-art and contribution

By and large, the 3D printing process briefly described above is well known but in many instances it is not yet adequately optimised and the influence of a variety of parameters hinder a large-scale production basis. For example, the intensity and direction of the UV light has no standard protocol [2], so the definition of an optimal disposition of the light sources can prove essential in minimising the polymerisation times, hence the whole tissue formation times as a whole. This work intends to ground the choice of selected polymerisation parameters to a rational basis. To achieve this, the relevant Physics of what happens after the melted bio-ink is deposited has been represented through multi-physics Finite Element simulations, where the kinetics of polymer cross-linking has been coupled with finite deformation formulations. Viscoelastic behaviour during polymerisation has also been accounted for. To deal with the highly non-linear differential equations representing the problem, a parametrised custom Finite Element variational formulation has been implemented. The relevant outputs from these simulations, e.g. the time-space maps of the polymer degree of conversion $p(\mathbf{r}, t)$ and bulk modulus $E_b(\mathbf{r}, t)$, have served as input data for modelling the successive phase of cell growth and tissue formation (see the presentation of Gaziano, P. et al., given in this minisymposium). Figure 1 shows an example of the distribution of light $I(\mathbf{r})$ within a polymer (treated as a Neo-Hookean medium with no viscoelastic effects) that causes the conversion of the initially present monomers into polymer chains $p(\mathbf{r})$.

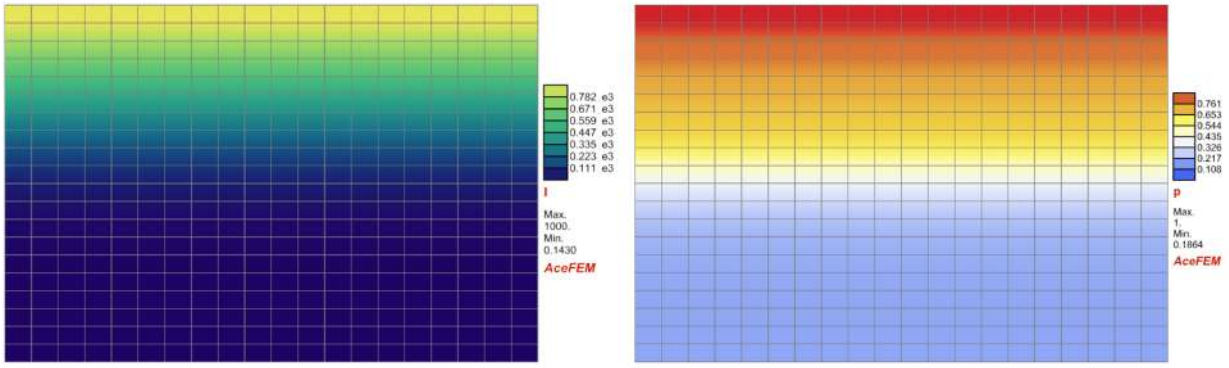


Figure 1: Light intensity attenuation (left) and degree of conversion (right) in a medium where UV lights activates polymerisation.

References

[1] Post M J *et al.* Scientific, sustainability and regulatory challenges of cultured meat. Nature Food 1.7 (2020).

[2] Wu J, *et al.* Evolution of material properties during free radical photopolymerization. Journal of the Mechanics and Physics of Solids (2018).

[3] Long K N *et al.* Photomechanics of light-activated polymers. Journal of the Mechanics and Physics of Solids (2009).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Phase-field modelling of cell motility within hydrogel scaffolds

Gaziano Pierfrancesco*, **Marino Michele***

* Department of Civil Engineering & Computer Sciences (DICII)
University of Rome "Tor Vergata", Rome, Italy
e-mail: gaziano@ing.uniroma2.it, m.marino@ing.uniroma2.it

Abstract: The present work addresses the development of a computational model to describe cell motility in bioprinted scaffolds for tissue engineering applications. Cell migration is treated as an advective/diffusive process modelled via the phase-field approach. Governing equations of the phase-field model are coupled with transport equations introduced to model the different chemo-biological mechanisms involved in the process, such as scaffold degradation, chemoattractant-induced cell-cell signaling pathways, as well as nutrient diffusion through the construct and its consumption by cells.

Keywords: Tissue growth, Cell motility, Phase-field model, Chemotaxis, Culture medium optimization

1 Introduction

Tissue engineering is a rapidly evolving field which has the potential to revolutionize many fields like medicine, by recreating tissues that can be effectively employed to replace lost or damaged tissues, or the food sector, by producing in laboratory meat destined for food use without the need for slaughtering animals [1].

Tissue growth is achievable only if cells are encapsulated within hydrogel scaffolds which provide them a mechanically supportive environment, at the same time guaranteeing cells viability by mimicking the extracellular matrix in which they are naturally immersed [1]. Tissue growth within bioprinted scaffolds is the result of a multifactorial process comprising cell differentiation, cell proliferation and/or migration, extracellular matrix (ECM) production, production and assembly of ECM and cells in a functional form. In particular, successful formation of neotissue is strictly related to cell motility, which in turn is dictated by several factors, such as: *i)* spatiotemporal changes of cellular microenvironment due to scaffold degradation; *ii)* chemical stimuli induced by other neighbouring cells triggering specific cell-cell signalling pathways; *iii)* proper transportation of growth factors, oxygen, nutrients, and waste in/out of the constructs.

The quality and quantity of the final product can be optimized only by finely tuning all the relevant variables involved in the process. However, optimization of process parameters is unlikely to be feasible through trial-and-error approaches, since the nature of the tests would lead to long lead times and potentially prohibitive costs. Numerical models of cell motility and tissue growth can be used, as they represent a relatively fast and low-cost alternative to successfully and effectively simulate *in-vitro* experiments. With this background, in this work a novel numerical model is developed with the aim of describing cell motility within a polymeric scaffold up to the event of mutual adhesion and fusion, considering precursor muscle cells (myoblasts) and PEG-fibrinogen-based hydrogels as a case study.

2 Materials and methods

The mathematical description of the afore-introduced mechano-chemo-biological mechanisms involves chemical reactions and diffusive/advective processes. The problem is tackled by means of a phase-field description of cell domains, which reformulates the moving boundary problem of collective cell migration as partial-differential equations defined over a known and fixed computational domain. [3]. The model accounts for the twofold nature of collective cell crawling in hydrogels, which consists in the superposition of a directed movement and many random turnings, resulting in a quasi-Brownian motion called persistent random motion (PRM) [2]. The directed motion is driven by chemoattractant substances expressed by neighbouring cells and sensed by membrane proteins (chemotaxis), as well as by variations of local substrate stiffness (durotaxis). Cell motility is modulated by the uptake of nutrients consumed by cells, and coupled with the mechanical response of the construct, in turn affected by polymer degradation over time. The previous features have been described through transport equations for the involved chemical species (nutrient and chemoattractant).

Present multi-field model has been implemented in a numerical framework based on a finite element (FE) formulation. Customized codes, comprising the implementation of a personalized quadrilateral FE with bi-linear isoparametric Lagrange shape functions, have been developed in Wolfram Mathematica, combining numeric and symbolic strategies.

3 Results and conclusions

Numerical results highlight the role of the nutrient and chemoattractant availability in the construct, as well as of the interplay between scaffold degradation and tissue growth. The developed computational framework is a first step towards a predictive tool for tissue growth in bioprinted scaffolds. The digital twin of the process will be coupled with a sensor platform based on optic fibers that allows to gain detailed information on the heterogeneous properties of scaffolds as produced during bioprinting. The integrated *in-vitro*/*in-silico* model will be exploited as an optimization strategy for the culture of bioprinted constructs in bioreactors, with the aim of maximizing neotissue formation.

References

[1] F. Berthiaume, T. J. Maguire, M. L. Yarmush, Tissue engineering and regenerative medicine: history, progress, and challenges, Annual review of chemical and biomolecular engineering 2 (2011), 403–430.

[2] D. Campos, V. M´endez, I. Llopis, Persistent random motion: Uncovering cell migration dynamics, Journal of theoretical biology 267 (4) (2010), 526–534.

[3] A. Moure, H. Gomez, Phase-field modeling of individual and collective cell migration, Archives of Computational Methods in Engineering 28 (2) (2021), 311–344.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A multiscale model of aneurysm development in the Marfan mouse aorta

Lauranne Maes* **and Nele Famaey***

* Department of Mechanical Engineering
KU Leuven
Leuven, Belgium
e-mail: lauranne.maes@kuleuven.be, nele.famaey@kuleuven.be

Abstract: In order to elucidate the complex interplay of factors leading to thoracic aortic aneurysm development in Marfan syndrome, a multiscale adaptive model is proposed, including a model of cellular regulation and a model of aortic tissue adaptation. Elastin degradation and the resulting aortic dilatation is predicted in wildtype mice, untreated Marfan mice and Marfan mice treated with losartan and enalapril. The results show good correspondence with experimental diameter measurements.

Keywords: Marfan syndrome, Multiscale adaptive model, Thoracic aortic aneurysm, Aorta growth and remodeling

1 Introduction

Marfan syndrome is a connective tissue disorder caused by a mutated fibrillin-1 gene. Its most life-threatening consequence for affected patients is the development of thoracic aortic aneurysms. There is currently no consensus on the pathophysiological origin of elastin degradation in the tissue, associated with aortic dilatation. Current hypotheses are related to AngII signaling, TGFβ signaling and endothelial dysfunction [1]. In order to further elucidate the complex interplay of these pathways and their effects at the tissue level, a multiscale model of the Marfan mouse aorta, including cellular regulation on the one hand, and tissue adaptation on the other hand, is proposed.

2 Methods

The cell-scale model is a network of protein signaling and gene expression and the tissue-scale model predicts evolving arterial wall composition. Both models are run alternately, considering a remodeling period of 240 days or time steps.

At the tissue-scale, a mixture of elastin and collagen is considered. Constant turnover of collagen is assumed, while elastin is gradually degrading according to $\dot{\phi}^{elas} = -\phi^{elas} k_d \Delta MMP$ with $\Delta MMP = \frac{y_{MMP} - y_{MMP,WT}}{y_{MMP,WT}}$, and where ϕ^{elas} is the fraction of intact elastin, k_d is a degradation rate parameter, y_{MMP} is a normalized concentration of elastin-degrading proteinases and WT refers to a wildtype control. At every time step, mechanical equilibrium is ensured using Laplace's law for pressurized cylinders with intraluminal pressure P, inner radius r_i and wall stress $\sigma_{\theta\theta}$.

The cell-scale model is a network model as shown on figure 1A. Every node in the network takes a value between 0 and 1 and node interactions are either activatory (green edges) or

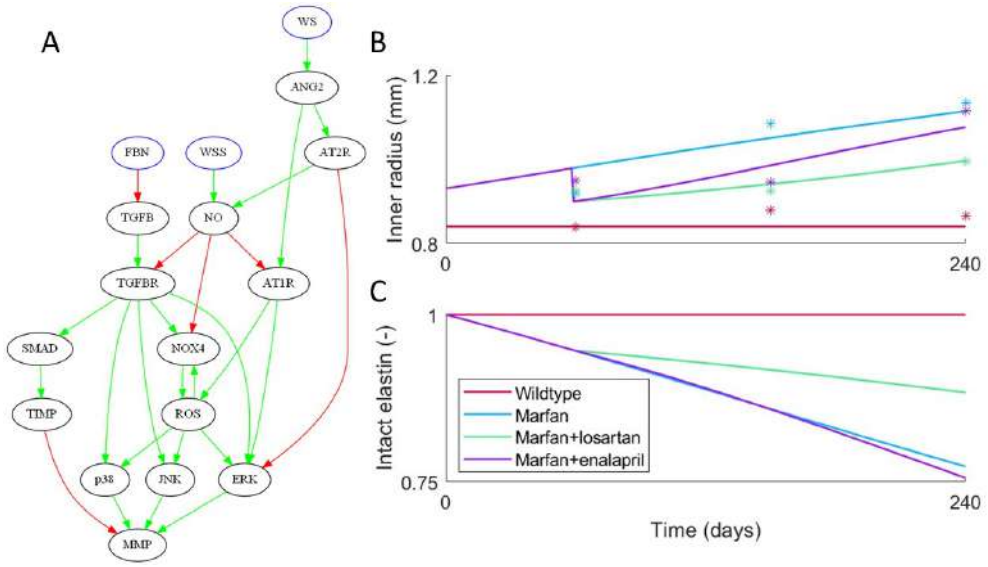


Figure 1: (A) Cell-scale network model. (B) Model inner radii over time compared to experiments [2]. (C) Model intact elastin fractions over time.

inhibitory (red edges). In order to calculate y_{MMP}, downstream node values are calculated as the average of their Hill-transformed upstream nodes. As indicated in blue in the figure, the network takes as inputs y_{FBN}, y_{WS} and y_{WSS}, where y_{FBN} represents the fraction of produced fibrillin-1, compared to the wildtype case, $y_{WS} = 1 - \frac{\sigma_{\theta\theta,WT}}{\sigma_{\theta\theta}}$ and $y_{WSS} = \left(\frac{r_{i,WT}}{r_i}\right)^3$.

Four cases predicting mouse aortic wall adaptation are considered, including a wildtype control case, and three Marfan mouse cases with 50% fibrillin-1, of which one untreated, one treated with losartan (inhibition of AT_1R) and one treated with enalapril (inhibition of AngII). Both drugs also are assumed to bring the intraluminal pressure, increased with 15% in Marfan mice [2], back to the wildtype level. In both treated cases, treatment started at day 60.

3 Conclusions

Figures 1B and 1C show the results of the four different cases. The model was calibrated to match experimental results on wildtype and $Fbn1^{C1039G/+}$ mice [2], as represented with stars on the figure. As is also observed experimentally, both tested drugs acutely reduce the wall diameter, while only losartan successfully reduces aneurysm formation on the longer term.

References

[1] Asano K, Cantalupo A, Sedes L, Ramirez F. Pathophysiology and Therapeutics of Thoracic Aortic Aneurysm in Marfan Syndrome. Biomolecules 2022;12(1):128.

[2] Verbrugghe P, Verhoeven J, Clijsters M, Vervoort D, Schepens J, Meuris B, Herijgers P. The Effect of a Nonpeptide Angiotensin II Type 2 Receptor Agonist, Compound 21, on Aortic Aneurysm Growth in a Mouse Model of Marfan Syndrome. J Cardiovasc Pharmacol 2018; 71(4):215-222.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Bearing/Pull-through Failure Envelope of Composite Joints: Novel Experimental Setup and Numerical Validation

A. Volpi[*], C. Furtado[*], R. F. Pinto[†], F. Danzi[*], G. Catalanotti[‡], F. J. Queirós de Melo*, P. P. Camanho*

[*] Department of Mechanical Engineering (DEMEC); INEGI
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: cfurtado@fe.up.pt

[†] proMetheus
Instituto Politécnico de Viana do Castelo
Faculdade de Engenharia, Universidade do Porto
Viana do Castelo, Portugal

[‡]Escola de Ciências e Tecnologia
Universidade de Évora
Évora, Portugal

Abstract: Current industry practice to connect composite structural panels still relies on the extensive use of bolted joints. However, due to their anisotropic nature, composite materials joining techniques represent a true design challenge, as their behaviour can change with, e.g. layup, material, geometry and environmental conditions. For this reason, the behaviour of composite bolted joints has been the subject of research studies for many years. Particular focus has been given to in-plane and out-of-plane performance of mechanically fastened composites. However, in real-life applications, e.g. for L-junctions and single lap joints of thin laminates, mechanically fastened joints are subject not only to pure bearing or pure pull-through, but have to sustain a combination of both loading scenarios [1,2]. Here, a novel test rig for determining the failure envelope of composite fastened joints under combined bearing and pull-through loading conditions is designed, tested and validated. The proposed device is compatible with a standard testing machine and captures the critical interactions between the two loading mechanisms for pull-through to bearing ratios ranging from 0.2 up to 0.8, allowing the characterization of the behaviour of composite joints under realistic loading scenarios. The multiaxial failure envelope for a carbon-fibre-based composite laminate is obtained experimentally and the performed tests are shown to fall within the limit values obtained for the pure bearing and pure pull-through loading conditions, obtained following well-established ASTM standards [3,4]. High-fidelity finite element simulations [5] are used to support the validation of the test methodology: the ability of the fixture to maintain a constant mixed load ratio during the whole test was numerically confirmed and a detailed analysis of the failure modes provided further insights into the main degradation mechanisms occurring during the experiments. A very good agreement between the numerical and experimental results is obtained for the entire failure envelope, with the numerical predictions falling between +-10% relative errors, further validating the constitutive modelling predictive capabilities.

Keywords: Composite Materials, FEM, Bolted joints, Damage Models

References

[1] J. Ekh, J. Schon, Composites Science and Technology 65 (6) (2005)

[2] G. M. Pearce, C. Tao, Y. H. Quek, N. T. Chowdhury, Composite Structures 187 (2018)

[3] ASTM D7332/D7332 M Standard Test Method for Measuring the Fastener Pull-Through Resistance of a Fiber-Reinforced Polymer Matrix Composite.

[4] ASTM D5961/D5961M Test Method for Bearing Response of Polymer Matrix Composite Laminates.

[5] P. Camanho et al., Mechanics of Materials 59 (2013) 36–49.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Data-driven microstructure-generator for high-fidelity analyses of unidirectional composite laminates

Silva R.[*], Danzi F.[*], Furtado C. [*], Lopes I. [*], Fanteria D. [†], Camanho P.P. [*]

[*] Department of Mechanical Engineering (DEMEC); INEGI
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: fdanzi@inegi.up.pt

[†] Faculty of Civil and Industrial Engineering of Pisa
Pisa, Italy

Abstract: Nowadays, micromechanical finite element analyses are a well-established technique to investigate the early-stage damage mechanisms of composite materials and to predict their homogenized mechanical properties. State-of-the-art high-fidelity simulations typically include consistent constitutive equations for the fibres and the matrix, the presence of the interfaces and, lately, the effect of voids and of the curing process [1]. Less emphasis is typically given to the fibre distribution itself [2]. In this work, the focus is given to the definition of a data-driven workflow for the generation of statistically equivalent fibre distributions for the simulation of composite systems. Unidirectional composites realized with different manufacturing processes are here investigated. More in detail, an hand-layup thermoset material cured in the autoclave is compared with a thermoplastic system consolidated in the hot press. Micrographs of the cross-section are analysed and the positions of fibres identified via digital-image analyses. Local and global statistical spatial descriptors including the nearest-neighbour distribution and the nearest-neighbour-orientations are then used for the fiber spatial distribution characterization. Statistically equivalent RVEs are then generated using the obtained descriptors and their mechanical response under different loading conditions investigated.

A set of linear elastic analyses is used to identify correlations between the fibre distribution and the resulting composite elastic properties. The matrix is then endowed with an elasto-plastic damageable model while the cohesive zone model technique is used to reproduce the failure in the fibre/matrix interface. The final results point out how different manufacturing processes induce a directionality in the microstructure distributions whose effect on the material degradation can not be considered as negligible.

Keywords: Composite Materials, FEM, Statistical distributions, Damage Models

References

[1] F. Danzi and D. Fanteria and E. Panettieri and M.C. Mancino. A numerical micro-mechanical study on damage induced by the curing process in carbon/epoxy unidirectional material. Comp. Struct., Vol. 210, 2019.

[2] F. Husseini and J. Pineda and E. Stapleton. Generation of artificial 2-D fiber reinforced composite microstructures with statistically equivalent features. Comp. Part A., Vol. 164, 2023J. Ekh, J. Schon, Composites Science and Technology 65 (6) (2005)

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Static bending and free vibration of Euler-Bernoulli beams using Fragile Point Method

Abinash Malla[1], **Sundararajan Natarajan** [2]

[1] Department of Mechanical Engineering
Indian Institute of Technology Madras
Chennai, 600036, India
e-mail: me21s014@smail.iitm.ac.in

[2] Department of Mechanical Engineering
Indian Institute of Technology Madras
Chennai, 600036, India
e-mail:snatarajan@smail.iitm.ac.in

Abstract: In this paper, the recently introduced Fragile Points Method (FPM) is extended to study the static bending and free vibration of Euler-Bernoulli beams. The beam kinematics is based on Euler-Bernoulli theory and based on assumptions that plane cross-sections of the beam remain plane and perpendicular to the deformed beam. The salient feature of the FPM is that it is a truly meshless method that employs simple local point-based polynomial test and trial functions, unlike element-based trial and test functions. The distinguishing feature is that, unlike the traditional Galerkin framework, the polynomial test and trial functions are discontinuous (piece-wise continuous over the global domain) that are derived by employing the generalized finite difference method. Further, as the trial and test functions are discontinuous, the continuity requirement imposed by the continuous Galerkin framework is circumvented. The discontinuous trial and test functions lead to inconsistency, to alleviate this, we employ numerical flux corrections inspired by the discontinuous Galerkin method. The efficiency and robustness of the approach are demonstrated with a few standard benchmark examples.

Keywords: Discontinuous Galerkin method, Fragile Points Method, Functionally graded material plate, Continuous Galerkin method, Generalized Finite Difference Method, Numerical Flux Correction

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A 2.5D hybrid SBM-MFS methodology for acoustic wave propagation problems

Fakhraei Javad*, Arcos Robert†, Pàmies Teresa † and Romeu Jordi†

* Acoustical and Mechanical Engineering Laboratory (LEAM)
Universitat Politècnica de Catalunya (UPC)
Terrassa (Barcelona), Spain
e-mail: javad.fakhraei@upc.edu

†Acoustical and Mechanical Engineering Laboratory (LEAM)
Universitat Politècnica de Catalunya (UPC)
Terrassa (Barcelona), Spain
e-mail: robert.arcos@upc.edu

†Acoustical and Mechanical Engineering Laboratory (LEAM)
Universitat Politècnica de Catalunya (UPC)
Terrassa (Barcelona), Spain
e-mail: teresa.pamies@upc.edu

†Acoustical and Mechanical Engineering Laboratory (LEAM)
Universitat Politècnica de Catalunya (UPC)
Terrassa (Barcelona), Spain
e-mail: jordi.romeu@upc.edu

Abstract: In this paper, a novel two-and-a-half dimensional hybrid singular boundary method-method of fundamental solutions (2.5D hybrid SBM-MFS) methodology to deal with exterior acoustic wave propagation problems is proposed and studied. The methodology is mainly developed to solve problems with complex boundary geometry in where the well-known boundary/geometric singularities of corner and sharp edge types are included in the boundary. The proposed methodology models the complex parts of the boundary with the SBM approach using so-called origin intensity factors for arisen singularities of the fundamental solutions employed, and the smooth parts with the MFS method. The feasibility, validity and accuracy of this hybrid scheme are tested in the framework of two case studies involving the radiation problems of an infinitely long pulsating circular cylinder in one case and an infinite pulsating square shape object as second case, in where the method is assessed and compared with the available analytical solutions, the 2.5D SBM and 2.5D MFS methods. The detailed comparison performed demonstrates that the 2.5D hybrid SBM-MFS methodology not only remedies severe numerical instabilities delivered by the 2.5D MFS in complex boundary geometries, but also significantly enhances the accuracy delivered by the 2.5D SBM.

Keywords: Singular Boundary Method, Method of Fundamental Solutions, 2.5D Modelling, Hybrid Scheme, Origin Intensity Factor, Acoustic Wave Propagation

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Robustness study of a hybrid SBM-MFS methodology for the simulation of acoustic and elastodynamic problems

Arcos, Robert[*,†], Clot, Arnau[*,†], Hassan, Liravi[*], Fakhraei, Javad[*] and Conto, Kenny F.[*]

[*] Acoustical and Mechanical Engineering Laboratory (LEAM)
Universitat Politècnica de Catalunya (UPC)
c/ Colom, 11, 08222 Terrassa (Barcelona), Spain
e-mail: robert.arcos@upc.edu, arnau.clot@upc.edu, hassan.liravi@upc.edu, javad.fakhraei@upc.edu, kenny.fernando.conto@upc.edu

[†] Serra Húnter Fellow
Universitat Politècnica de Catalunya (UPC)
Spain
e-mail: robert.arcos@upc.edu, arnau.clot@upc.edu

Abstract: The meshless methods, as an alternative to the mesh-based approaches, started to capture the interest of a broader community of researchers over the last decades. In meshless methods, there is no inherent reliance on a particular mesh topology, resulting in simpler formulations and computational implementation procedures of the method. Over the last few years, numerous studies have been carried out on novel meshless approaches to solve acoustic and elastodynamic problems. The method of fundamental solution (MFS) and the singular boundary method (SBM) are popular approaches in this category. A recently developed method that combines the MFS and the SBM for the simulation of two-dimensional (2D) and two-and-a-half-dimensional (2.5D) problems in acoustics and elastodynamics is deeply studied in the present work. Studies on the amount of virtual sources with respect to collocation points, the distribution of MFS and SBM sources or the placement of the MFS sources will be presented. These studies have been carried out in the context of various benchmark examples accounting for regular and complex geometries, deeply studying the accuracy, efficiency of the novel hybrid method in comparison with reference analytical solutions of the addressed problems. From the results obtained, robustness of the hybrid SBM-MFS method is discussed and guidelines to ensure it are proposed.

Keywords: Numerical simulation, Meshless methods, Wave propagation, MFS, SBM, BEM, ...

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

An efficient three-dimension piled foundation model based on the singular boundary method for solving ground-borne vibration problems.

Kenny F. Conto*, Robert Arcos† *, Arnau Clot† * and Hassan Liravi*

* Acoustical and Mechanical Engineering Laboratory (LEAM)
Universitat Politècnica de Catalunya (UPC)
c/Colom 11, Terrassa (Barcelona), Spain.
e-mail:{kenny.fernando.conto, hassan.liravi}@upc.edu

† Serra Húnter Fellow
Universitat Politècnica de Catalunya (UPC)
Barcelona, Spain.
e-mail:{robert.arcos, arnau.clot}@upc.edu

Abstract: This paper proposes a new efficient three-dimensional (3D) building-soil model for predicting low-amplitude ground-borne vibration of piled structures in radiation and scattering cases. The model accounts for the Singular Boundary Method (SBM) for computing the half-space reaction. The soil is strongly coupled with the piled foundation, which is modelled as bars or Euler-Bernoulli beams for accounting for axial and lateral movements, respectively. The robustness of the model is discussed by comparing, in a three-story building example, its results with the ones obtained by the 3D FEM-BEM. The comparison reveals that the robustness and efficiency of the proposed methodology provide accurate results without decreasing its computational efficiency

Keywords: piled foundation, multi pile, singular boundary method (SBM), meshless method, soil-structure interaction

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

An energy based material model for Shape Memory Alloys

Cem Erdogan*, Tobias Bode* and Philipp Junker*

* Leibniz Universität Hannover, Fakultät für Maschinenbau,
Institute of Continuum Mechanics (IKM),
Hannover, Deutschland
e-mail: erdogan@ikm.uni-hannover.de

Abstract:

The particular property of shape memory alloys, as compared to other metals with possible martensitic microstructure, is their significantly higher sensitivity of the martensite-austenite phase transformation to thermal and mechanical loads. This property offers shape memory alloys special applications in practice. However, the behavior of shape memory alloys is difficult to be predicted solely based on experience due to their complex behaviour. Consequently, the simulation of shape memory alloy structures is of high importance. Taking into account the thermomechanical coupling effect, we present a rate-independent material model which allows the determination of the microstructural state in terms of volume fractions of crystallographic phases. The material model is based on energetic quantities and is derived by applying the Hamilton principle. The model has proven to be accurate and robust, which is demonstrated by simulation results for structural devices made of shape memory alloys.

Keywords: shape memory alloy, phase transformation, thermo-mechanical coupling, variational modelling, finite element method

1. Introduction

The mechanical behaviour of shape memory alloys dependens on the phase composition of the grains. There are several approaches to calculate the volume fractions of martensite and austenite in grains. In [1] a robust, accurate and fast material model has been presented. It is based solely on energetic quantities, which lead to universal applicability. However, the material model is difficult to handle in mathematical terms, so the active set strategy must be used which is known to be complex to implement. To solve this open problem, the present material model was further developed.

2. Material model

To derive the evolution equations of the present material model, we use the principle of the minimum of the dissipation potential, as described in [1],[2] and [3]. This principle states

$$\mathcal{L} = \dot{\Psi}(\boldsymbol{\varepsilon}, T, \boldsymbol{\lambda}, \boldsymbol{\alpha}) \; + \; \Delta(\dot{\boldsymbol{\lambda}}, \dot{\boldsymbol{\alpha}}) + cons(\dot{\boldsymbol{\lambda}}, \dot{\boldsymbol{\alpha}}) \rightarrow \operatorname*{stat}_{\dot{\boldsymbol{\zeta}}} \tag{1}$$

The vector $\dot{\boldsymbol{\zeta}}$ collects the rates of the internal Variables, which are the rodrigues paramter $\dot{\boldsymbol{\alpha}}$ and the volume fraction of the crystallographic phases $\dot{\boldsymbol{\lambda}}$. By evaluation of the stationarity conditions of the Lagrangian (1), the evolution equations

$$\dot{\boldsymbol{\lambda}} = \left[-\frac{\partial \psi}{\partial \boldsymbol{\lambda}} + \left(\frac{1}{n} \sum \frac{\partial \psi}{\partial \lambda_i} \right) \right] \rho_\lambda \tag{2}$$

$$\dot{\boldsymbol{\alpha}} = \left[-\frac{\partial \psi}{\partial \boldsymbol{\alpha}} + \left(\frac{\partial \psi}{\partial \boldsymbol{\alpha}} \cdot \boldsymbol{\alpha} \right) \boldsymbol{\alpha} \right] \rho_\alpha \tag{3}$$

can be derived when we chose $\Delta := r_\lambda \left\|\dot{\boldsymbol{\lambda}}\right\| + r_\alpha \|\dot{\boldsymbol{\alpha}}\|$ with the consistency parameters $\rho_\lambda := \left\|\dot{\boldsymbol{\lambda}}\right\|/r_\lambda$ and $\rho_\alpha := \|\dot{\boldsymbol{\alpha}}\|/r_\alpha$. The model is set when we define a Helmholtz free energy function. Here, we chose the following approach, cf. [1], which we expand by a penalty term

$$\Psi = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{Q}^{\boldsymbol{T}} \cdot \overline{\boldsymbol{\eta}} \cdot \boldsymbol{Q}) : \bar{\mathbb{C}} : (\boldsymbol{\varepsilon} - \boldsymbol{Q}^{\boldsymbol{T}} \cdot \overline{\boldsymbol{\eta}} \cdot \boldsymbol{Q}) + \sum \frac{\kappa_0}{\lambda_i^2(\lambda_i - 1)^2} \tag{4}$$

The reorientation is described in terms of the rotation matrix $\boldsymbol{Q} = \boldsymbol{Q}(\boldsymbol{\alpha})$. Furthermore, the volume fractions $\boldsymbol{\lambda}$ are expressed by $\boldsymbol{\chi}$ and related by a sigmoid function in order to increase the stability of the model. Consequently, the equation (2) can be extended to

$$\dot{\boldsymbol{\chi}} = \left(\frac{\partial \boldsymbol{\lambda}}{\partial \boldsymbol{\chi}}\right)^{-1} \left[-\frac{\partial \psi}{\partial \boldsymbol{\lambda}} + \left(\frac{1}{n}\sum \frac{\partial \psi}{\partial \lambda_i}\right)\right] \rho_\lambda \tag{5}$$

3. Numerical results

The material model is tested on a stent in Abaqus. In the first step, the representative surface is moved in radial direction so that the stent is crimped. In the second step, the displacement state of the representative surface is blocked in the radial direction and the temperature of the stent is increased from -10 °C to 37.5 °C. The resultant volume fraction distribution of the austenite phase is given in Figure 1.

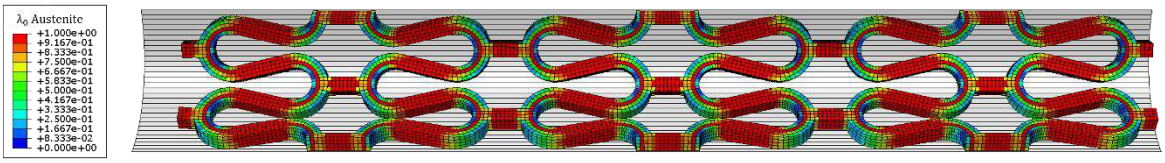


Figure 1: Distribution of the volume fraction of the austenite phase within one quarter of a stent

In areas exposed to strong tensile and compressive stresses due to bending, the volume fraction of the austenite phase is low. Consequently, in the neutral fibre, the volume fraction of the austenite phase is high.

4. Conclusions

As a result of the described mathematical modifications inequality constraints are no longer accounted for as in [1], [2] and [3] and thus, the active set strategy is no longer necessary. The numerical simulation results are reasonable and robust, as even the calculation of a complex boundary value problem with contact conditions, thermo-mechanical loading and large strain energy converges in an Abaqus user material implementation.

References

[1] Junker P. An accurate, fast and stable material model for shape memory alloys. Smart Mater. Struct. 23(11), 115010 (2014)

[2] Junker P,Jaeger S, Kastner O, Eggeler G, Hackl K: Variational prediction of the mechanical behaviour of shape memory alloys based on thermal experiments. Journal of the Mechanics and Physics of Solids 80: 86-102 (2015)

[3] Junker P: A novel approach to orientation distribution functions for modeling and simulation of polycrystalline shape memory alloys. International Journal for Numerical Methods in Engineering 98(11): 799-818 (2014)

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical investigation of fiber suspensions in ball probe rheometers

Florian Gerland[*], Thomas Schomberg[*] and Olaf Wünsch[*]

[*] Department of Fluid Dynamics
Faculty of Mechanical Engineering, University of Kassel, Germany
e-mail: fluiddynamics@uni-kassel.de

Abstract: Fibers made from shape memory alloys (SMA) are capable of transforming from a compact to an elongated geometry by applying heat. When mixing fresh concrete, fibers with a compact, for e.g. ellipsoidal, geometry are added to the fresh concrete, which can improve the rheological properties of fresh concrete compared to conventional rod-shaped fiber-reinforced concrete. After activation of the shape memory effect, the fibers return to their common rod-like shape and develop their residual flexural strength-increasing effect after solidification of the concrete. The imprinted geometry of the SMA fibers significantly influences the rheological behavior of the fresh concrete. The rheological properties are investigated in ball probe rheometers. It is known that not only the fiber geometry but also the fiber orientation in suspensions significantly determines the rheological behavior. However, measurements of fiber suspensions with ball probe rheometers show only minimal orientation effects in the M-Ω measurement curves, although a temporally extended orientation process has been observed visually during the measurements. This contribution investigates the flow of a fiber suspension in a ball probe rheometer by numerical simulations to explain how this apparent contradiction occurs. The findings can be applied to derive rheological parameters of fresh fiber reinforced concrete from measurements in ball probe rheometers.

Keywords: Concrete rheology, Bingham plastic, fiber orientation, cell model, orientation evolution equation

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

The influence of latent heat on inductive heating of shape memory alloy fibers

Stefan Descher*, Philipp Krooß†, Detlef Kuhl* and Sebastian Wolf*,

* Institute of Structural Mechanics
University of Kassel
Mönchebergstr. 7
Kassel, Germany
e-mail: descher@uni-kassel.de

† Institute of Materials Engineering
Metallic Materials
University of Kassel
Mönchebergstr. 3
Kassel, Germany
e-mail: krooss@uni-kassel.de

Abstract: Ultra High Performance Concrete is highly dense concrete filled with steel fibers, and well known for its outstanding mechanical behavior in the civil engineering community. Further improvement is possible using pre-stretched shape memory alloy fibers instead. They enable introducing an internal prestess state by activation of the one way effect, which leads to fiber contraction. As a result, there is tension in the fiber, and largely compression in its proximity if the fiber geometry is chosen properly. For activation, the fibers need to be heated up until a microstructure transformation from martensite to austenite takes place. Because heating up large parts is not energy efficient, this is done by an induction heater. The present work deals with the efficiency of the inductive heating in the above described process. It considers the endothermic character of the martensite-austenite transformation, geometric and electromagnetic parameters, as well as an elastomeric fiber coating. The non-isothermal phase transition is modeled empirically, based on data from Differential Scanning Calorimetry. Parameter studies are performed for an axisymmetric single fiber case with an induction coil using the Finite-Element-Method.

Keywords: Shape Memory Alloys, Electromagnetism, Differential Scanning Calorimetry, FEM

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A Multi-Scale Framework for the Modelling of Intergranular Fracture in Polycrystalline Materials under Slip Plasticity and Martensitic Transformation

Vieira de Carvalho, M.*†, Rodrigues Lopes, I. A.† and Andrade Pires, F. M.†

† Department of Mechanical Engineering (DEMec)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mails: mvcarvalho@fe.up.pt, ilopes@fe.up.pt, fpires@fe.up.pt

Abstract: In this contribution, a large strains multi-scale computational framework is formulated to model the behaviour of polycrystalline materials under slip plasticity, mechanically-induced martensitic transformation and intergranular fracture. With this framework, it is possible to study de impact of these lattice dissipative phenomena on the intergranular crack propagation mechanism.

The so-called transformation-induced plasticity (TRIP) effect, that occurs in the 3rd generation of advanced high-strength steels (AHSS), increases the strain-hardening capacity of multi-phase steels. Additionally, previous research on the impact of this effect on the fracture toughness of metallic materials also shows that the formation of martensite at the crack tip can lead to improved mechanical properties, such as fracture toughness.

The cohesive zone model is combined with the constitutive model proposed by [1] to model intergranular fracture in metallic materials that undergo crystal-plasticity-like phenomena, such as slip plasticity and martensitic transformation. A multi-scale model that relates discontinuous microstructures to a continuous macroscopic domain is also developed using the method of multi-scale virtual power (MMVP) [2], which includes micro-cracks and inertial effects in the micro-scale equilibrium problem. Moreover, to homogenise traction-separation laws and fracture properties, a large strain fracture-based computational homogenisation procedure is introduced. It is derived from a crack-based Hill-Mandel principle [3] and is capable of accurately defining the crack domain and compute the crack homogenised quantities.

Keywords: Finite Element Method, Multi-Scale, Crystal Plasticity, Martensitic Transformation, Intergranular Fracture, Method of Multi-Scale Virtual Power.

References

[1] de Carvalho, M. V., de Bortoli, D., and Andrade Pires, F. M. (2022). Consistent modeling of the coupling between crystallographic slip and martensitic phase transformation for mechanically induced loadings. *International Journal for Numerical Methods in Engineering*, 123(14):3179–3236.

[2] Blanco, P. J., Sánchez, P. J., de Souza Neto, E. A., and Feijóo, R. A. (2016). Variational Foundations and Generalized Unified Theory of RVE-Based Multiscale Models. *Archives of Computational Methods in Engineering*, 23(2):191–253.

[3] Turteltaub, S. and Suárez-Millán, R. (2020). Energetically-consistent multiscale analysis of fracture in composites materials. *European Journal of Mechanics - A/Solids*, 84:104079.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A second-order computational homogenisation approach for investigating porous materials

Wanderson F. dos Santos[*,†], Igor A. Rodrigues Lopes[†,#], Sergio P. B. Proença[*] and Francisco M. Andrade Pires[†]

[*] Department of Structural Engineering (SET)
Sao Carlos School of Engineering, University of Sao Paulo
Sao Carlos, Brazil
e-mail: wanderson_santos@usp.br
e-mail: persival@sc.usp.br

[†] Department of Mechanical Engineering (DEMec)
Faculty of Engineering, University of Porto
Porto, Portugal
e-mail: ilopes@fe.up.pt
e-mail: fpires@fe.up.pt

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

Abstract: This work presents a second-order computational homogenisation formulation based on the *Method of Multi-scale Virtual Power* [1] for investigating the constitutive behaviour of porous materials. The macro-scale continuum is described by a second gradient theory and the micro-scale is modelled by the concept of Representative Volume Element (RVE) with the classical first-order continuum mechanics. The framework allows the construction of three different sets of micro-scale kinematic constraints: minimal (lower bound), periodic and direct (upper bound). The kinematic constraints are imposed over the RVE by the Lagrange multiplier method, and the macroscopic stress tensors can be recovered by expressions written from the Lagrange multipliers values. An analogous framework was proposed in the context of composites by Lopes and Pires [2], whose formulation is not suitable for investigating porous media. On the other hand, the generality of the new formulation allows the consideration of voids inside the RVE and also on its external contour. More specifically, the strategy presented by Rocha et al. [3] to study voids on RVE contour in the context of first-order homogenisation was extended to second-order homogenisation. This approach is interesting for computing the macroscopic constitutive behaviour of solids with higher strain gradients and high curvatures. In particular, deformations modes involving bending or torsion can be captured. Furthermore, it is worth mentioning that the developed formulation can be explored in the numerical simulation of the constitutive behaviour of a wide range of porous solids, for instance, cellular and lattice structures as well as metamaterials.

Keywords: Second-Order Computational Homogenisation, Finite Strains, Second Gradient Continuum, Method of Multi-Scale Virtual Power, Porous Solids.

References

[1] Blanco PJ, Sánchez PJ, de Souza Neto EA, Feijóo RA. Variational Foundations and Generalized Unified Theory of RVE-Based Multiscale Models. Archives of Computational Methods in Engineering 2016;23:191–253.

[2] Rodrigues Lopes IA, Andrade Pires FM. Formulation and numerical implementation of a variationally consistent multi-scale model based on second-order computational homogenisation at finite strains for quasi-static problems. Computer Methods in Applied Mechanics and Engineering 2022;392:114714.

[3] Rocha FF, Blanco PJ, Sánchez PJ, de Souza Neto EA, Feijóo RA. Multi-scale modelling of arterial tissue: Linking networks of fibres to continua. Computer Methods in Applied Mechanics and Engineering 2018;341:740–787.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Virtual elements in microstructural crystalline environments

Christoph Böhm[*], **Michele Marino**[†] **and Peter Wriggers**[*]

[*] Institute of Continuum Mechanics
Leibniz Universität Hannover
An der Universität 1, 30823 Garbsen, Germany
e-mail: {boehm,wriggers}@ikm.uni-hannover.de

[†] Department of Civil Eng. and Computer Science
University Rome Tor Vergata
Via del Politecnico 1, 00133 Rome, Italy
e-mail: m.marino@ing.uniroma2.it

Abstract: Crystalline microstructures exhibit in general a heterogeneous environment at microscopic length scales. This entails the request of a (partially) fine discretization to maintain an accurate response for quantities obtained by computational homogenization approaches using finite elements. An immediate consequence is the rise of computational costs that is tied to the number of equations that have to be solved for finding a solution of the boundary value problem under consideration. Contrary, the real quantities of interest feature still (only) an integral relation over the entire microscopic domain. In this regard, the Virtual Element Method (VEM) proved to be advantageous by portraying grain-structures with an element-to-grain approach (one element equals one grain) [1, 2, 3]. This property is provided by its general formulation that allows for arbitrary shapes, see [4]. The objective of this contribution is to show extensions of the virtual element formulations to the modelling of such environments under consideration of computational homogenization approaches.

Keywords: Virtual Element Method (VEM), Crystalline Microstructure, Computational Homogenization

1 Constitutive framework, computational approach and computational homogenization

The problem under consideration is a solid domain with a possibly coupled electro-magneto-mechanical response. It is governed by the Gauss laws of electro-/magneto-statics as well as the balance of linear momentum in a linearized kinematic framework, following [5], and reads

$$\operatorname{div}(\boldsymbol{\sigma}) + \boldsymbol{f} = \boldsymbol{0}, \quad \operatorname{div}(\boldsymbol{D}) = q, \quad \operatorname{div}(\boldsymbol{B}) = \boldsymbol{0}. \tag{1}$$

Hereby, $\boldsymbol{\sigma}$ is the stress (tensorial quantity of $2nd$ order), $\boldsymbol{f}$ is a body force, applied to the solid, $\boldsymbol{D}$ denotes the vector of electric displacement and $\boldsymbol{B}$ is the magnetic flux density vector. div is the divergence operator. Following [2], an energetic coupled response function $\psi(\boldsymbol{\varepsilon}, \boldsymbol{E}, \boldsymbol{H}; \boldsymbol{a})$ is formulated as a quadratic relation in terms of the linearized strain $\boldsymbol{\varepsilon}$ and the electric (resp. magnetic) field $\boldsymbol{E}$ (resp. $\boldsymbol{H}$). A directional dependent response for the crystallines at the microstructural level is introduced via a material preferred direction $\boldsymbol{a}$, see also [5].
Following [4], the construction of the virtual element relies on a split of the primary fields $\mathfrak{C}_h = \mathfrak{C}_\pi + (\mathfrak{C}_h - \mathfrak{C}_\pi), \mathfrak{C}_h = (\boldsymbol{u}_h, \phi_h, \varphi_h)$, with $\boldsymbol{u}_h$ being the displacement and ϕ_h (resp. φ_h) being the electric (resp. magnetic) potential. subscript $(\cdot)_\pi$ denotes a projected quantity. With the

particular choice for a low order ansatz it follows for the gradients of the projected fields

$$\nabla \mathfrak{C}_\pi|_E = \frac{1}{\|\boldsymbol{\Omega}_E\|} \sum_{F \in E} \sum_{\tau \in F} \int_{\boldsymbol{\Omega}_E} \mathfrak{C}_h \otimes \tilde{\boldsymbol{n}}_\tau \mathrm{d}\Gamma_F. \tag{2}$$

Hereby, Γ_F denotes the area of the specific face $F \in E$ and E denotes the particular virtual element i.e., the crystalline grain, with $V_E = \|\boldsymbol{\Omega}_E\|$ being its volume. $\tilde{\boldsymbol{n}}_\tau$ is a generalized unit normal vector to the triangle $\tau \in F$, pointing outwards of E. The approach to homogenization is based on the fundamental formulation of the generalized Hill-Mandel condition, see [5]. It ties a representative volume element (RVE) to the macroscopic material point $\boldsymbol{X}_M$. The

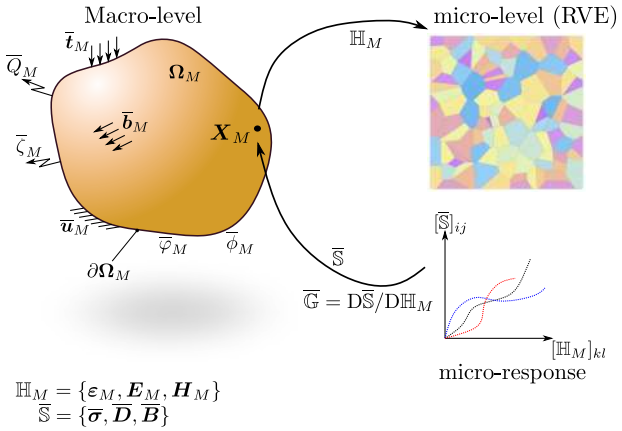


Figure 1: Schematic illustration of the localitzation of the micro-problem and its homogenization. Macroscopic quantities are indicated by $(\cdot)_M$, homogenized fields are summarized in $\overline{\mathbb{S}}$ and $\overline{\mathbb{G}}$.

solution to the homogenization problem is obtained via sensitivity analysis (see also [6]), extended to the formulation of virtual elements.

2 Conclusions

Results will turn out the advantage of VEM in a microstructural crystalline framework. VEM is able to predict accurate response in highly heterogeneous environments [2, 3]. Hereby, VEM is able to reduces the computational costs in hands with providing an increased flexibility for the discretization of grained microstructures.

3 Acknowledgements

CB and PW acknowledge funding by the German Research Foundation (DFG) within the framework of the collaborative research centre 1153 (SFB 1153), project number 252662854.

References

[1] Marino, M., Hudobivnik, B., & Wriggers, P. (2019). Computational homogenization of polycrystalline materials with the Virtual Element Method. *Computer Methods in Applied Mechanics and Engineering*, 355, 349-372.

[2] Böhm, C., Hudobivnik, B., Marino, M., & Wriggers, P. (2021). Electro-magneto-mechanically response of polycrystalline materials: Computational homogenization via the virtual element method. *Computer Methods in Applied Mechanics and Engineering*, 380, 113775.

[3] Böhm, C., Munk, L., Hudobivnik, B., Aldakheel, F., Korelc, J., & Wriggers, P. (2023). Virtual Elements for computational anisotropic crystal plasticity. *Computer Methods in Applied Mechanics and Engineering*, 405, 115835.

[4] Beirão da Veiga, L., Brezzi, F., Marini, L. D., & Russo, A. (2014). The hitchhiker's guide to the virtual element method. *Mathematical models and methods in applied sciences*, 24(08), 1541-1573.

[5] Schröder, J., Labusch, M., & Keip, M. A. (2016). Algorithmic two-scale transition for magneto-electro-mechanically coupled problems: FE2-scheme: Localization and homogenization. *Computer Methods in Applied Mechanics and Engineering*, 302, 253-280.

[6] Korelc, J., & Wriggers, P. (2016). Automation of Finite Element Methods. Springer.

Short Abstract for ECCOMAS YIC 2022

Descriptor-based microstructure characterization and reconstruction – fixed inclusion shapes vs. free voxel formulation

Paul Seibert, Markus Husert, Alexander Raßloff, Karl Kalina, Markus Kästner
Institute of Solid Mechanics, TU Dresden

Microstructure Characterization and Reconstruction (MCR) allows for (i) generating a plausible 3D computational domain from 2D information like a microscopy image, (ii) generating a set of statistical volume elements from a single representative example and (iii) augmenting microstructure datasets by sampling and interpolating in the descriptor space and subsequently reconstructing the corresponding structures. Two classes of reconstruction algorithms, descriptor-based and machine learning-based approaches, are distinguished and their advantages and disadvantages for computational materials engineering are compared.

After a formulation of the descriptor-based optimization problem, the differentiability of the same descriptors is recognized as a suitable measure for ensuring high efficiency by gradient-based optimization [1, 2]. Alternatively, restricting the microstructure to a composition of simple shapes like ellipsoids reduces the dimensionality of the optimization problem. In fact, these measures do not stand in conflict, but are combined by deriving and harnessing analytical formulations for different descriptors of non-overlapping ellipsoid distributions as well as their derivatives. This facilitates a geometrically restricted but drastically accelerated reconstruction procedure that is contrasted to the unrestricted voxel-based formulation regarding strengths, weaknesses and use-cases.

[1] Seibert, Ambati, Raßloff, Kästner, Reconstructing random heterogeneous media through differentiable optimization, COMMAT, 2021
[2] Seibert, Raßloff, Ambati, Kästner, Descriptor-based reconstruction of three-dimensional microstructures through gradient-based optimization, Acta Materialia, 2022
[3] Seibert, Raßloff, Kalina, Ambati, Kästner, Microstructure Characterization and Reconstruction in Python: MCRpy, IMMJ, 2022

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Refined modeling of the interaction of adjacent grains inside a Tungsten polycrystal

Guillaume Hanon, Laurent Delannay

Institute of Mechanics, Materials and Civil Engineering (IMMC)
UCLouvain
1348 Louvain-la-Neuve, Belgium
e-mail: guillaume.hanon@uclouvain.be & laurent.delannay@uclouvain.be

Abstract: Full-field predictions of the microscopic heterogeneity of stresses and strains across a polycrystalline aggregate may be predicted by implementing crystal plasticity theory either in a finite element code (CPFEM) or in a spectral (FFT) solver. When relying on a voxelized grid (or a brick-shaped FE mesh), the geometry of the model polycrystal does not conform exactly to the grain boundaries. In this study, an original strategy is adopted in order to model the interaction of adjacent grains along grain boundaries in spite of a non-conforming mesh. It is shown to predict accurately the GB stresses at a reduced computational cost.

Keywords: Crystal Plasticity, Element Finite Analysis, Microstructure, Voxel

1. Introduction

Ensuring structural integrity of Tungsten components in nuclear fusion reactors, as the ITER divertor [1], implies reliable estimates of Fatigue Indicator Parameters (FIPs) [2]. Accurate predictions of the stress raisers nearby grain boundaries (GB) may require applying crystal plasticity on highly refined FE meshes [3]. It may be tedious to generate meshes that conform to the complex geometry of GB networks, and the computational time also quickly increases. Different approaches have thus been proposed in order to limit inaccuracies induced by the use of a coarse or a non-conforming FE mesh. The method proposed here is suitable also when using a spectral (FFT) solver.

2. Method

A square periodical domain was meshed uniformly with brick-shaped elements (Fig. 1(b)). Then, a microstructure consisting of a periodic Voronoi tessellation of 100 grains was immersed [4]. Every element cut by a GB, was modelled as a bicrystal whereas a single crystal orientation was considered within every element fully inside a grain. The response of the bicrystal was computed by enforcing stress equilibrium and strain compatibility across the interface and by minimising the deformation of the two grains [5].

3. Results

The comparison of CPFEM on conforming (Fig. 1(a)) and non-conforming (Fig. 1(b)) meshes shows that the same level of accuracy is reached when predicting GB stresses and fatigue indicator parameters (FIPs). Moreover, the calculation time was drastically reduced with the non-conforming mesh. The average deformation of each bicrystal was somewhat closer to the macroscopic strain, which supports the main hypothesis of the ALAMEL multisite modelling scheme [5].

(a) (b)

Figure 1. Microstructure made of 100 Tungsten grains – (a): irregular mesh made of tetrahedrons and conforming to GB – (b): regular voxel mesh

4. Conclusions

The original approach proposed here predicts accurately GB stresses at a reduced computational cost. Ongoing research involves further assessment based on a comparison to experimental results. It would be also interesting to investigate the quality of the predictions of lattice rotation in the GB region with this new model as grains boundary interactions is critical in texture development.

Acknowledgements

Financial support for this work was provided by FNRS as well as Eurofusion. LD is mandated by FNRS, Belgium. Computational resources were provided by the supercomputing facilities of the UCLouvain (CISM/UCLouvain) and the Consortium des Équipements de Calcul Intensif en Fédération Wallonie Bruxelles (CÉCI) funded by the Fond de la Recherche Scientifique de Belgique (F.R.S.-FNRS) under convention 2.5020.11 and by the Walloon Region.

References

[1] Hirai, T., Panayotis, S., Barabash, V., Amzallag, C., Escourbiac, F., Durocher, A., ... & Uytdenhouwen, I. (2016). Use of tungsten material for the ITER divertor. *Nuclear Materials and Energy*, *9*, 616-622.

[2] Muth, A., John, R., Pilchak, A., Kalidindi, S. R., & McDowell, D. L. (2021). Analysis of Fatigue Indicator Parameters for Ti-6Al-4V microstructures using extreme value statistics in the HCF regime. *International Journal of Fatigue*, *145*, 106096.

[3] Delannay, L., Melchior, M. A., Signorelli, J. W., Remacle, J. F., & Kuwabara, T. (2009). Influence of grain shape on the planar anisotropy of rolled steel sheets–evaluation of three models. *Computational materials science*, *45*(3), 739-743.

[4] C. Geuzaine and J.-F. Remacle. *Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities*. International Journal for Numerical Methods in Engineering 79(11), pp. 1309-1331, 2009.

[5] Van Houtte, P., Delannay, L., & Kalidindi, S. R. (2002). Comparison of two grain interaction models for polycrystal plasticity and deformation texture prediction. *International Journal of Plasticity*, *18*(3), 359-377.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Composite Boxels with imperfect Interfaces (ComBI) with FFT-based solvers

Sanath Keshav*, Felix Fritzen* and Matthias Kabel†

*SC Simtech, Data Analytics in Engineering
University of Stuttgart, Germany
e-mail: {keshav,fritzen}@mib.uni-stuttgart.de

† Department Flow and Material Simulation,
Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM
Kaiserslautern, Germany
e-mail: matthias.kabel@itwm.fraunhofer.de

Abstract: Cohesive zones were first introduced to simulate the production of cracks caused by interfacial damage. However, the term is often used in a broader sense to refer to imperfect interfaces governed by constitutive traction separation laws. In unstructured finite element simulations, cohesive zones are discretized by specific interface conforming cohesive elements. The discretization of FFT-based methods is generally non-conforming to the interfaces; hence the classical interface cohesive elements cannot be employed. In this work, we propose a framework that is a generalization of composite boxels [Keshav, S. Fritzen, F. Kabel, M. 2022, Kabel, M et al. 2015] for interfacial damage modeling in FFT-based solvers. The special focus is on gathering the interface metadata from images using a novel image-based algorithm. An efficient implementation with a particular emphasis on numerical robustness is proposed. Numerical examples along with traction and stress field statistics comparing the proposed framework with unstructured finite element simulations are presented.

Keywords: Homogenization, Fast Fourier transform, composite boxel, cohesive zone modeling

References

[1] Keshav S., Fritzen F. & Kabel M. FFT-based homogenization at finite strains using composite boxels (ComBo). Comput Mech 71, 191–212 (2023).

[2] Kabel M., Merkert D., & Schneider, M. (2015). Use of composite voxels in FFT-based homogenization. Computer Methods in Applied Mechanics and Engineering, 294, 168-188.

[3] Leuschner M., Fritzen F. Fourier-Accelerated Nodal Solvers (FANS) for homogenization problems. Comput Mech 62, 359–392 (2018).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Inversely identifying material parameters for a multiscale framework to model creep deformation using Deep Material Networks

Argha Protim Dey*, Fabian Welschinger*, Matti Schneider†, Sebastian Gajek† and Thomas Böhlke †

* Robert Bosch GmbH,
Corporate Sector Research and Advance Engineering,
Robert-Bosch-Campus 1, 71272 Renningen, Germany
e-mail: arghaprotim.dey@de.bosch.com

† Institute of Engineering Mechanics (ITM),
Karlsruhe Institute for Technology (KIT),
Kaiserstraße 10, 76131 Karlsruhe, Germany
https://www.itm.kit.edu/

Abstract: The simulative characterization of the creep response of short-fiber reinforced thermoplastics (SFRTs) is complex due to the presence of multiple scales, both in space (due to the reinforcements) and in time (short- and long-term effects). To reduce the involved effort, computational multiscale approaches may be used to characterize these models experimentally. Since the various parameters of the model must be identified from experimental data, having proper microstructure and microscopic material models at hand does not speed-up the material characterization. In the current work, we perform an inverse parameter optimization of the matrix model of a SFRT using Deep Material Networks (DMN) in place of full-field simulations. Due to the substantial anisotropy and the extensive time scales involved, we are particularly interested in the long-term creep response of SFRTs, which presents unique difficulties for both experimental and simulation-based techniques. Furthermore, we are interested in a more generalized framework, wherein we use multiple trained DMNs to interpolate over different fiber orientation tensors and fiber lengths within the microstructure.

Keywords: Multiscale methods; Deep material network; Creep loading; Short-fiber reinforced thermoplastics.

1. Introduction

On the microstructural level for SFRTs, the matrix and fibers are modeled by separate constitutive material laws. We utilize a fully coupled plasticity and creep model for the matrix [1]. One approach would be to identify the material parameters based on experiments performed on pure matrix material and use the same parameters for FFT-based numerical homogenization [2]. This approach leads to inaccurate results since the change in mechanical properties of the matrix induced by the manufacturing process are not accounted for in the model. A direct and practical way to identify the material properties would be to use the experiments performed on the composite. This task would be daunting even if each simulation is run using the current state-of-the-art FFT-based computational homogenization [2]. It is particularly time-consuming when a large number of iterative cycles are involved. We suggest an alternative approach where we replace the micromechanical model with the deep material networks (DMN) [3,4,5], which is a data-driven homogenization technique. The DMNs can reproduce the highly non-linear creep models and offers a speed-up factor of 600 on average when compared to full-field simulations [6].

2. Calibration of coupled plasticity and creep law

2.1. Comparison with experiments for a single microstructure

The elastic, plastic and creep parameters are inversely identified using a DMN-based optimization subroutine for a representative microstructure [1]. The DMN simulations using the identified parameters are compared with the experimental results under creep loading in Fig. 1.

Fig. 1 shows that the overall elasto-plastic and creep response is well represented considering the range of stresses and time scales involved.

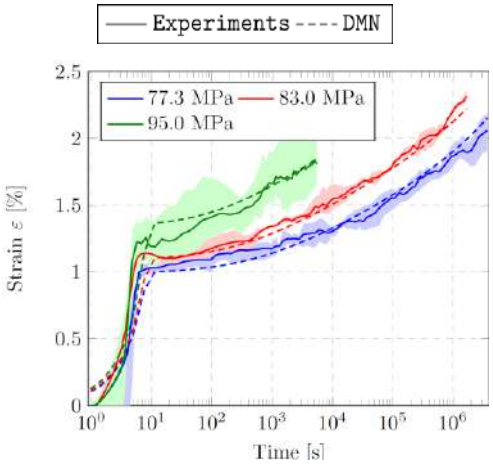


Figure 1. Experimental and simulation results with inversely identified parameters for creep loading.

2.2. Generalized framework for multiple microstructures

The extension of the inverse calibration workflow towards different materials involves the data generation and training of the DMN for each microstructure. We aim to circumvent this time consuming approach by interpolating over the two main variable parameters of the microstructural arrangement: fiber orientation tensor and fiber length. Several DMNs are trained over the interpolation space and a generalized material response for all microstructures within the space is obtained.

3. Conclusions

In this work, the inverse problem was solved using the DMN framework, and the experiments on the composite were utilized to determine the parameters for the constitutive model of the polymer matrix (in our instance, a fully coupled plasticity-creep law). We demonstrated that such a method can accurately describe the anisotropic response of the composite and accurately identify the material parameters of the matrix from the composite experiments. The interpolation over fiber orientation and fiber length makes the framework suitable for the calibration of various material models for different classes of SFRTs.

References

[1] Dey, A. P., Welschinger, F., Schneider, M., Gajek, S. & Böhlke, "Rapid inverse calibration of a multiscale model for the viscoplastic and creep behavior of short fiber-reinforced thermoplastics based on Deep Material Networks." *Int. J. Plast* 2022; 103484.

[2] Schneider, M. "A dynamical view of nonlinear conjugate gradient methods with applications to FFT-based computational micromechanics." *Comput. Mech.* 2020, vol. 66, 239–257.

[3] Gajek, S., Schneider, M. & Böhlke, T. "On the micromechanics of deep material networks." *J. Mech. Phys. Solids* 2020;142, 103984

[4] Liu, Z., Wu, C. T. & Koishi, M. "A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials." *Comput. Methods in Appl. Mech. Eng.* 2019; 345, 1138–1168.

[5] Liu, Z. & Wu, C. T. "Exploring the 3D architectures of deep material network in data-driven multiscale mechanics." *J. Mech. Phys. Solids* 2019; 127, 20–46.

[6] Dey, A. P., Welschinger, F., Schneider, M., Gajek, S. & Böhlke, T. "Training deep material networks to reproduce creep loading of short fiber-reinforced thermoplastics with an inelastically-informed strategy" *Arch. Appl. Mech.* 2022; 92, 2733–2755.

FFT-based homogenization of non-local damage and size effects in composite materials.

M. Magri[1], J. Segurado[2,3]

[1] MOX Laboratory, Department of Mathematics, Polytechnic University of Milan, Italy.

[2] Department of Materials Science, Technical University of Madrid, Spain.

[3] Fundación IMDEA Materiales, Madrid, Spain,.

The resulting strength and ductility of composite materials depends on the interplay between mechanisms operating at different length scales. As a result, prominent size effects – typically connected to the size of the reinforcements – are encountered in experiments. For instance, in particle reinforced metal matrix composites, it has been observed an increase in strength with decreasing particle size at a constant volume fraction of the reinforcement. In addition to that, the size of the particles influences the ductility of the composite material, although in this case bigger particles can increase or decrease the ductility depending on the dominant damage mechanism.

The numerical simulation of such size effects require the implementation of non-local mechanical models incorporating combined inelastic and damage theories. It this contribution, we present a non-local micro mechanical model based on (i) the incorporation of a lower-order strain gradient plasticity model and (ii) the application of an implicit gradient regularization technique to the Gurson-Tvergaard-Needleman ductile damage model for metals. Such an extended model is equipped with two length-scale parameters, one for each non-local extension, which modulate the size dependent character of the formulation.

The resulting model is a non-conventional mechanical problem consisting of three coupled partial differential equations. This problem is numerically solved via a purposely developed staggered algorithm that exploits the sequential usage of FFT-Galerkin and conjugate gradient based solvers. The resulting approach is robust and efficient allowing for the simulation of complex three dimensional micromechanical problems with millions of voxels and different phases. The numerical results show that the employed non-local extension of damage successfully suppresses the spurious grid dependence typical of (local) damage models. Moreover, the combined effect of damage and strain gradient plasticity is analyzed in the simulated size dependent homogenized response of such composites.

References

[1] M. Magri, S. Lucarini, G. Lemoine, L. Adam, and J. Segurado. An FFT framework for simulating non-local ductile failure in heterogeneous materials. COMPUT METHODS IN APPL MECH ENG, 380:113759, 2021.

[2] M. Magri, L. Adam, and J. Segurado. Particle size effects in ductile composites: An FFT homogenization study. J MECH PHYS SOLIDS, 160:104759, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Influence of fractal nature of pores on corrosion-driven fracture in cementitious materials

Pundir Mohit*, Angst Ueli* and Kammer David S.*

* Institute for Building Materials (IfB)
ETH Zurich, Switzerland
e-mail: mpundir@ethz.ch

Abstract: Corrosion-driven fracture in cementitious materials is a multi-scale and multi-physics problem. The mechanisms such as ionic diffusion, precipitation and stress development occur within the micropores of cementitious material. The micropores in cementitious material are highly complex and fractal. As a result, the study of corrosion-driven fracture relies heavily on approximating pore space and structure. This paper presents an FFT-based framework for solving corrosion-driven fractures within a fractal porous media, thus preserving pore shape and form. We show the capability of the FFT-based spectral method to resolve the multiple corrosion-driven mechanisms within a fractal porous microstructure. We analyze how approximating a fractal pore space influence different mechanisms and, consequently, the corrosion-driven fracture. Our results show the significance of persevering the pore shape as it affects the crack initiation and propagation and, therefore, the overall stresses developed within a microstructure.

Keywords: Corrosion-driven fracture, FFT-based approach, Ionic diffusion, Phase-field model

1 Introduction

Corrosion of reinforcement bars in concrete plays a significant role in determining a structure's durability and serviceability lifetime [1]. Corrosive species (Fe^{2+}, OH^-) diffuse through the pore space of cementitious material and chemically react to form corrosion products ($Fe(OH)_2$, $Fe(OH)_3$) within the pore space. These precipitates grow within the confined pore space and exert pressure on the solid phase, which leads to fracture initiation and, ultimately, to a structure's deterioration. Therefore, the pore structure and the pore space in cementitious material play a crucial role from the initiation of corrosion until the crack nucleation. Due to the complex nature of the pore structure in cementitious material: pore sizes range from nanometers to micrometres, and the fractal nature of pores, approaches proposed in the literature usually simplify the complex pore space to overcome computational difficulties. Either with the representation of fractal volumes or with the simulation of processes within fractal spaces. Therefore, the pore characteristics' influence on corrosion-driven mechanisms is inadequately understood. In this paper, we present an FFT-based spectral integral framework [2] to simulate various corrosion-driven mechanisms: ionic diffusion, stress development due to the growth of precipitates, and internal cracking. We use the proposed framework to characterize the influence of pore spaces' fractal nature on corrosion-driven fracture initiation within a microstructure.

2 Methods

We present a Fourier-based framework to simulate the ionic diffusion within the pore space of a microstructure and couple it with thermodynamic modelling of chemical reactions to quantify the precipitate formation and, consequently, porosity decrease. We employ a phase-field approach within the FFT framework to simulate crack initiation and propagation. A diffused representation of crack allows characterization of how a micro-structure evolves (change in porosity) due to internal cracking. Finally, we employ an FE-FFT-based multiscale approach to upscale the microscale mechanisms, such as ionic diffusion, precipitate growth and crack initiation, to the macroscale.

3 Results

We analyze in depth the differences that arise in corrosion-driven mechanisms due to approximating a fractal space as Euclidean space, such as cylinders or spheres. We show that preserving the pore shape is crucial. Approximating a fractal pore shape with Euclidean shapes, as done in multiscale modelling and homogenization approaches [3], leads to differences in the diffusion of ions and the rate at which precipitates grow within a microstructure. We show that even if total porosity is preserved in the approximation of fractal pore space, as usually done in multiscale approaches, the differences arise in how the stresses develop locally within a micro-structure, which significantly affects the failure stress as well as the post-failure mechanisms within a microstructure.

4 Conclusions

We present an FFT-based spectral integral framework for corrosion-driven processes (*e.g.*, diffusion and mechanical) that is computationally efficient, and its extension to a multiscale approach is straightforward. We show the significance of the fractal nature of pores and how its approximation underestimates various physical mechanisms. The present framework, along with the insights from this study, thus can be used to understand better the role of the fractal nature of pore spaces, an aspect often neglected or crudely approximated, on corrosion-driven mechanisms and similar multi-physical mechanisms in the cementitious material.

References

[1] Ueli M. Angst. “Challenges and opportunities in corrosion of steel in concrete”. en. In: *Materials and Structures* 51.1 (Feb. 2018), p. 4.

[2] H. Moulinec and P. Suquet. “A numerical method for computing the overall response of nonlinear composites with complex microstructure”. en. In: *Computer Methods in Applied Mechanics and Engineering* 157.1 (Apr. 1998), pp. 69–94.

[3] F.-J. Ulm. “Is concrete a poromechanics material? - A multiscale investigation of poroelastic properties”. en. In: *Materials and Structures* 37.265 (Nov. 2003), pp. 43–58.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Variationally consistent computational homogenization of chemo-mechanical properties of nano-porous battery electrode materials

David Rollin[1,*], Fredrik Larsson[2], Kenneth Runesson[2], and Ralf Jänicke[1]

[1] Institute of Applied Mechanics
Technische Universität Braunschweig
Braunschweig, Germany
e-mail: {d.rollin; r.janicke}@tu-braunschweig.de

[2] Division of Material and Computational Mechanics
Chalmers University of Technology
Gothenburg, Sweden
e-mail: {fredrik.larsson; kenneth.runesson}@chalmers.se

Abstract:

In Li-ion batteries various multiphysics processes occur on multiple length scales. A promising new type of battery is the structural battery which stores energy as well as it bears mechanical loads, allowing for significant mass savings. In this case, the interaction of the mechanical properties and the electro-chemical processes is of particular interest. One crucial aspect is the swelling of the electrode material due to lithium storage during dis/charging.

In a structural battery realized as a carbon fiber reinforced polymer, the positive electrode can be designed as a fiber coating. Such an electrode material typically consists of particles embedded in a porous binder matrix filled with an electrolyte. For this type of material, we aim at developing a model describing the chemo-mechanical coupling mechanisms.

To date, no 3D imaging data is available. Therefore, microstructures investigated in this study have been generated artificially as stochastically representative volume elements. The concept of variationally consistent computational homogenization is applied to investigate the processes across the scales. The base for our work is a linearized chemo-mechanical model which will be extended to account for reaction kinetics on the particle surfaces. From the fine-scale model, a two-scale problem is derived by applying first order homogenization.

Keywords: Li-ion battery, variationally consistent computational homogenization, chemo-mechanical coupling

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A Fully-nonlocal Quasicontinuum Approach for Predicting Fracture in Periodic 3D Metamaterials

Kevin Kraschewski*, Gregory P. Phlipot† and Dennis M. Kochmann*

* Mechanics & Materials Lab, Department of Mechanical and Process Engineering
ETH Zürich
Zurich, Switzerland
e-mail: kkraschewski@ethz.ch

† Divison of Engineering and Applied Science
California Institute of Technology
Pasadena, United States of America
e-mail: gphlipot@caltech.edu

Abstract: With the progress of advanced additive manufacturing techniques, fabricated periodic truss lattices may contain millions of periodically arranged unit cells (UCs). Given the ongoing up-scaling of manufacturing processes, the prediction of the robustness of the macroscale response in the presence of imperfections, e.g., pre-cracks, is crucial. To predict the mechanical response of large structures, continuum finite element simulations are too costly, so that homogenization becomes the method of choice. Classical hierarchical homogenization techniques rely on the assumption of a separation of scales. When the separation of scales breaks down, e.g., in the case of fracture mechanics, such techniques fail. Therefore, we present a concurrent multiscale technique, viz. a fully-nonlocal quasicontinuum (QC) multi-lattice formulation based on a conforming mesh. Our QC formulation is applied to trusses described by a linear elastic, geometrically nonlinear corotational beam representation, which captures significant nonlinearity and localization effects in fully-resolved regions, while efficiently treating the remaining simulation domain through a coarse-graining technique. We show that our method can efficiently predict the fracture toughness of truss lattices, while using a fraction of the computational resources of comparable fully-resolved simulations.

Keywords: Metamaterial, Multiscale modelling, Homogenization, Finite elements, Fracture

1 Introduction

The fracture of linear elastic continua is well-characterized by the toughness K_{IC}. However, recent studies suggest that this is not necessarily the case for 3D mechanical metamaterials [1], even in the linear regime. It was shown that not only the crack size but also the triaxiality affect the fracture toughness. They further showed that the effect of the triaxiality and the number of unit cells over the crack flank can be captured via a single paramater, which is related to the T-stresses. These observations suggest that the commonly reported metamaterial scaling laws of the form

$$\frac{K_{IC}}{\sigma_f \sqrt{l}} = D\bar{\rho}^d, \tag{1}$$

with σ_f and $\bar{\rho}$ being the failure stress and relative density, respectively, are insufficient to characterize fracture in 3D truss-based metamaterials. To investigate, among others, fracture in periodic trusses, we extend a concurrent multiscale technique, known as the fully-nonlocal quasicontinuum (QC) multi-lattice formulation on a conforming mesh [2].

2 The Mixed-Order Quasicontinuum Method

We consider periodic truss lattices $\Omega = \{\mathcal{P}, \mathcal{E}\}$, which consist of sets of beam junctions $\mathcal{P}$ (in the following referred to as nodes) and truss members $\mathcal{E}$. The truss lattices are constructed by repeating a unit cell (UC) along predefined directions. We collect all degrees of freedom (DOFs) of a UC at location $\boldsymbol{X}_i$ in a vector $\tilde{\varphi}(\boldsymbol{X}_i) = [\boldsymbol{\varphi}^1(\boldsymbol{X}_i), \ldots, \boldsymbol{\varphi}^{n_B}(\boldsymbol{X}_i)]$, with $\boldsymbol{\varphi}^j(\boldsymbol{X}_i)$ being the vector of generalized DOFs of node j within a UC and n_B being the number of nodes of truss members only connecting nodes within UCs. To reduce computational costs, we approximate the DOFs of Ω by a reduced subset and approximate the total potential energy similarly to a quadrature rule. Therefore, we choose N_{rep} representative unit cells (RepUCs, with $N_{rep} \ll N$, where N is the total number of UCs in the lattice) and apply an interpolation scheme for the remaining set. We further introduce a sampling rule to approximate the total potential energy, which is based on a weighted sum of the strain energy densities W_s over N_s sampling UCs. This is summarized by

$$\tilde{\boldsymbol{\varphi}}(\boldsymbol{X}_u) \approx \sum_{r=1}^{N_{rep}} N_r(\boldsymbol{X}_u)\, \tilde{\boldsymbol{\varphi}}_r, \qquad \mathcal{I}(\boldsymbol{\varphi}) \approx \sum_{s=1}^{N_s} \omega_s W_s(\tilde{\boldsymbol{\varphi}}) - \mathcal{L}_s(\tilde{\boldsymbol{\varphi}}). \tag{2}$$

Here, $N_r(\boldsymbol{X}_u)$ and $\boldsymbol{\varphi}_r$ are the shape functions evaluated at UC locations $\boldsymbol{X}_u$ and the DOFs of the RepUCs, respectively. This representation allows us to define a fully-resolved region, i.e., every UC is a RepUC and a sampling UC, where we recover the accuracy of fully discrete calculations, while coarse-graining is achieved by selecting only a few RepUCs. Previous studies [2] suggest that using first-order interpolation results in an overestimation of the energy densities for bending-dominated lattices, such as the hexagon, due to overconstraining the lattice. Therefore, we extend the method of Phlipot and Kochmann [2] to include higher-order interpolation in coarse-grained regions, while keeping the simplicity of first-order elements in the fully-resolved regions.

3 Conclusions

We present an efficient multiscale framework to investigate fracture in periodic truss-based metamterials. The method is equivalent to a fully-discrete calculation in some regions, e.g., near the crack flank, where every UC is also a RepUC, but is efficient in coarse-grained regions. Results include the fracture toughness of a variety of stretching- and bending-dominated truss lattices.

References

[1] Angkur Jyoti Dipanka Shaikeea, Huachen Cui, Mark O'Masta, Xiaoyu Rayne Zheng, and Vikram Sudhir Deshpande. The toughness of mechanical metamaterials. *Nature Materials*, 21(3):297–304, March 2022.

[2] Gregory P. Phlipot and Dennis M. Kochmann. A quasicontinuum theory for the nonlinear mechanical response of general periodic truss lattices. *Journal of the Mechanics and Physics of Solids*, 124:758–780, March 2019.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Characterization of TPMS foams using multiscale techniques

Ana Pais[*], Jorge Lino Alves[*] and Jorge Belinha[†]

[*] Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: anapais@fe.up.pt; falves@fe.up.pt

[†] Department of Mechanical Engineering
School of Engineering, Polytechnic of Porto
Porto, Portugal
e-mail: job@isep.ipp.pt

Abstract: Multiscale modelling refers to an approach in which analysis of the material is conducted at one length scale but the outcomes of the analysis are referent to several properties of the material at another length scale.

The use of numerical homogenization techniques allows for significant savings in computational time. Often in composites it is not necessary and inneficient to model the entirity of the structure of the composite. Instead, only a representative region is chosen to model all the consitutents of the composite.

This approach can be extended to lattice materials, by simplifying the assumption, where the composite presents two or more phases (fiber and matrix), and the lattice will only present one phase, being the rest a void phase. The mechanical properties of the lattice material are given as a function of their relative density.

This work evaluates the elastic and plastic properties of two cellular structures based on TPMS, the gyroid and the primitive surface. The study allowed to obtain correlations for the relative Young's modulus and relative yield stress as a function of the relative density which correlated well to experimental data found in the literature.

Keywords: TPMS, Homogenization, Gyroid, Primitive, Cellular materials

Acknowledgements

The authors truly acknowledge the funding provided by LAETA, under project UIDB/50022/2020 and the doctoral grant SFRH/BD/151362/2021 financed by the Portuguese Foundation for Science and Technology (FCT), Ministério da Ciência, Tecnologia e Ensino Superior (MCTES), with funds from the State Budget (OE), European Social Fund (ESF) and PorNorte, under the MIT Portugal Program.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

On the modeling of the interfaces in PC/ABS ternary blends

Alexandre C. Amaro[1] and A. Francisca C. Alves [2] and Bernardo P. Ferreira [3] and Miguel V. Carvalho [4] and F. M. Andrade Pires [5]

1 Department of Mechanical Engineering (DeMec), Faculty of Engineering of University of Porto, Porto, Portugal, up201806113@up.pt

2 Department of Mechanical Engineering (DeMec), Faculty of Engineering of University of Porto, Porto, Portugal, afalves@fe.up.pt

3 School of Engineering, Brown University, 184 Hope St, Providence, RI 02912, U.S.A., bernardo_ferreira@brown.edu

4 Department of Mechanical Engineering (DeMec), Faculty of Engineering of University of Porto, Porto, Portugal, mvcarvalho@fe.up.pt

5 Department of Mechanical Engineering (DeMec), Faculty of Engineering of University of Porto, Porto, Portugal, fpires@fe.up.pt

Abstract: The PC/ABS polymer blend is one of the most successful commercial polymer blends, finding its main applications in the automotive sector and consumer electronics. The relevance of this blend lies in the combination of both the excellent thermal and mechanical properties of polycarbonate (PC), and the toughness of acrylonitrile-butadiene-styrene (ABS) – itself a binary blend of styrene-acrylonitrile (SAN) and polybutadiene (rubber).

Depending on the loading conditions and the morphology of the blend, different deformation mechanisms control the response of the material. Among these deformation mechanisms, one can highlight the internal particle cavitation of the rubber particles and the debonding at the interface between the PC matrix and ABS particles [1]. As an alternative to the continuum modeling of such phenomena, often based on phenomenological assumptions, multi-scale modeling based on computational homogenization arises as an effective way to predict the thermomechanical response of these blends. Besides the proper establishment of a representative volume element and the constitutive description of both material phases, it is expected that accounting for the explicit modeling of the PC/ABS interfaces is crucial to achieve accurate predictions.

In the present contribution, a microstructure generator program is developed to efficiently generate the PC/ABS representative volume elements incorporating interface elements around the ABS particles. The PPR potential-based cohesive model [2] is selected to characterize the behavior of the interface elements, and the homogenized thermomechanical response of the PC/ABS blends is inferred through first-order hierarchical multiscale analyses based on computational homogenization. Several numerical analyses are conducted to assess the influence of explicitly accounting for the interface phase in the blend's microstructure effective response.

Keywords: Multi-scale modeling, PC/ABS polymer blends, Interfaces, Microstructure generation, Finite element analyses

References

[1] Seelig, T. and Giessen, E. (2007). Effects of microstructure on crack tip fields and fracture toughness in PC/ABS polymer blends. International Journal of Fracture, 145(3):205–222.

[2] Park, K. and Paulino, G. H. (2012). Computational implementation of the PPR potential-based cohesive model in ABAQUS: Educational perspective. Engineering Fracture Mechanics, 93:239–262.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modelling coupled chemo-mechanical fracture in DAMASK

Roongta Sharan*, Shanthraj Pratheek†, Diehl Martin†† and Roters Franz*

* Max-Planck-Institut für Eisenforschung
Max-Planck-Straße 1
40237 Düsseldorf, Germany
e-mail: s.roongta@mpie.de

† University of Manchester
Department of Materials
United Kingdom
e-mail: pratheek.shanthraj@manchester.ac.uk

†† Department of Computer Science & Department of Materials Engineering
Celestijnenlaan 200a
3001 Leuven, Belgium
e-mail: martin.diehl@kuleuven.be

Abstract: Loading of crystalline structural materials during service usually involves interactions between multiple physical phenomena which influence the material microstructure and properties. Understanding the connection between loading conditions, microstructure, and material properties is a labour intensive process. Computer simulations are therefore used to understand and predict the microstructure-property relationships across multiple length scales by modelling the phenomenon of interest and solving it using advanced numerical methods. In this work, we present a model to study hydrogen-assisted grain boundary fracture. It involves the coupling of diffusion (chemistry), mechanics and phase field damage at the microstructural scale. Complexity arises due to the different time and length scales associated with solute diffusion and the fracture process. Therefore, a modelling and solving strategy is introduced to study such coupled multi-scale phenomenon. The model is implemented in Düsseldorf Advanced Material Simulation Kit (DAMASK), an open source, multi-physics crystal plasticity software, with the capability and flexibility to perform and analyze complex multi-field simulations. Its modular structure allows for solving of different field equations, for example, mechanical, thermal, damage diffusion equations using solvers provided by the PETSc numerical library.

Keywords: hydrogen, grain-boundary fracture, multi-physics, multi-scale, open-source software.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Assessing the Effectiveness of Tensor-Train-Based Preconditioners For Numerical Homogenization

Lennart Risthaus[*†], **Matti Schneider**[*]

[*] Institute of Engineering Mechanics
Karlsruhe Institute of Technology
Karlsruhe, Germany

[†]e-mail: lennart.risthaus@kit.edu

Abstract: To reduce the effort of characterizing heterogeneous materials experimentally, computational homogenization approaches are frequently used. Particularly effective are approaches based on the fast Fourier transform (FFT), which use FFT to evaluate a constant-coefficient preconditioner. In the work at hand, we exploit using the Tensor Train (TT) format to efficiently store the preconditioner without relying upon FFT. Such an approach enables us to treat different boundary conditions than periodic.

Keywords: Computational Homogenization, Multi-scale Materials, Low-rank Methods

1 State of the Art

Fast Fourier Transform (FFT)-based homogenization methods allow to compute the effective properties of a microstructure swiftly. Periodic boundary conditions are intrinsic to FFT-based solution methods, such as the classic approach by Moulinec and Suquet [1]. Periodic boundary conditions provide a middle-ground between the overestimation of the effective properties by Dirichlet boundary conditions and the underestimation of the properties by Neumann boundary conditions, as realized by Hill [2] in the 1960's and corroborated later on. Handling other boundary conditions requires some additional effort for FFT-based solution methods. Dirichlet, Neumann and periodic boundary conditions were studied for finite element discretizations, by using subdomains of an periodic FFT-based solution field, or by a Discrete Cosine (DCT) or Discrete Sine Transform (DST) [3]. For the case of periodic boundary conditions, a multitude of discretization schemes were proposed and to solve the discrete system of equations, various solution methods were explored. The pioneering solution method was the so-called Basic Scheme [1] which can be interpreted as a preconditioned gradient descent scheme [4]. We refer to the review [5] for further insight into discretization schemes and solution methods.

On regular grids, many entries of the differential operators for finite differences are redundant. Additionally, the arrays succumb to the curse of dimensionality where the number of array entries grows exponentially in the dimension. A low-rank method, known as the matrix product state in quantum physics, is the tensor train (TT) format, introduced by Oseledets [6]. The TT format has certain benefits over other low-rank formats such as the possibility of performing algebraic operations while keeping the result in a low-rank format. As certain algebraic operations – while retaining the TT format – increase the TT ranks, the TT format allows for an efficient recompression of the TT tensors [6]. The effectiveness of applying this

approach to real-world problems with low dimension $d = 2, 3$ – such as problems of numerical homogenization – can be increased significantly by employing the so-called quantics tensor train [7] format. The low-rank approximation of the inverse of the Laplacian was studied for stochastic homogenization [8].

2 Contributions

In the work at hand, we assess the effectiveness of a low-rank TT-based preconditoner [8] for various boundary conditions in numerical homogenization of heat conduction using a finite difference discretization on large-scale microstructures. By inversion of the multidimensional Laplacian via the TT format, we obtain Green's operator as a preconditioner for the accelerated gradient descent scheme used to solve the Lippmann-Schwinger equation. Different (mixed) boundary conditions are treated naturally within this framework by adjusting the used preconditioner. We compare our results against results obtained by application of the conventional preconditioner using the Fourier transform. Additionally, we assess the convergence and the performance of the TT-based preconditioner and highlight the advantages and disadvantages of this novel approach.

References

[1] Moulinec H and Suquet P. A fast numerical method for computing the linear and nonlinear mechanical properties of composites. Comptes Rendus de l'Académie des Sciences. Série II 1994;318:1417–23.

[2] Hill R. Elastic properties of reinforced solids: Some theoretical principles. J Mech Phys Solids 1963;11:357-372

[3] Swarztrauber PN. The Methods of Cyclic Reduction, Fourier Analysis and the FACR Algorithm for the Discrete Solution of Poisson's Equation on a Rectangle. SIAM Rev 1977;19:490–501.

[4] Brisard S and Dormieux L. Combining Galerkin approximation techniques with the principle of Hashin and Shtrikman to derive a new FFT-based numerical method for thehomogenization of composites. Comput Methods Appl Mech Eng 2012;217-220:197–212.

[5] Schneider M. A review of nonlinear FFT-based computational homogenization methods. Acta Mech 2021;232:2051–100.

[6] Oseledets IV. Tensor-Train Decomposition. SIAM J Sci Comput 2011;33:2295–317.

[7] Khoromskij BN. O(dlog N)-Quantics Approximation of N-d Tensors in High-Dimensional Numerical Modeling Constr Approx 2011;34:257–80.

[8] Khoromskij BN and Khoromskaia V. Fast solution of three-dimensional elliptic equations with randomly generated jumping coefficients by using tensor-structured precondition- ers. Numer Linear Algebra Appl 2022;e2477.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Local reduced modes for multiscale simulations of pattern-transforming mechanical metamaterials

Doškář Martin*, Rokoš Ondřej†, Peerlings Ron†, Geers Marc† and Zeman Jan*

* Department of Mechanics
Faculty of Civil Engineering, Czech Technical University in Prague
Prague, Czech Republic
e-mail: Martin.Doskar@cvut.cz

† Department of Mechanical Engineering
Eindhoven University of Technology
Eindhoven, Netherlands

Abstract: Metamaterials derive their constitutive behaviour from a carefully designed microstructural geometry, which in the case of pattern-transforming mechanical metamaterials can undergo significant changes during loading. Computational homogenization is a way to capture the effective metamaterial's response without resorting to a macroscopic model with fully resolved microstructural details; yet the computational cost of this approach remains high.

Reduced-order modelling is a successful strategy for reducing computational time of problems with low-dimensional parameterisation (such as the first-order homogenization); however, the solution manifold of pattern-transforming microstructures cannot be easily covered by a linear subspace of reduced modes mainly due to the presence of several buckling modes.

We propose a reduced-order modelling scheme that builds on local reduced bases and capitalizes on a specific structure of the metamaterial's Representative Volume Elements (RVEs). First, we perform polar decomposition and solve the underlying Boundary Value Problem for a macroscopic right stretch tensor $\mathbf{U}^{\mathrm{M}}$ instead of the macroscopic deformation gradient $\mathbf{F}^{\mathrm{M}}$. Next, we utilize RVE symmetries and transform the right stretch tensor $\mathbf{U}^{\mathrm{M}}$ such that it follows a selected symmetric part of the RVE. Note that this step also significantly reduces the offline training phase. Finally, we distinguish local states bases on whether the microstructure remains in the original configuration or any of the patterns has been triggered. We utilize a classifier based on a neural-network to predict which of the local bases should be chosen given the prescribed $\mathbf{U}^{\mathrm{M}}$. To further accelerate the calculations, we supplement the reduced basis with optimized quadrature rules.

We illustrate the proposed scheme and report its efficiency for macroscale simulations of metamaterials composed of square and hexagonal arrangements of circular holes.

Keywords: Mechanical metamaterials, Computational homogenization, Reduced-order modelling, Local bases

Acknowledgements*

This research was funded by the Czech Science Foundation through project No. 19-26143X.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Predicting post-bifurcated patterns of architectured materials using group theory

Rachel Azulay*, Christelle Combescure† and Justin Dirrenberger*

* Laboratoire PIMM
Arts et Metiers, CNRS, Cnam, HESAM Université, 75013 Paris, France
e-mail: rachel.azulay@ensam.eu, justin.dirrenberger@ensam.eu

† Univ. Bretagne Sud, UMR CNRS 6027, IRDL, F-56100 Lorient, France
Saint-Cyr Coetquidan Military Academy, CReC, 56380 Guer, France
e-mail: c.combescure@st-cyr.terre-net.defense.gouv.fr

Abstract: Numerous studies concerning the crushing of honeycombs have shown that the symmetry of the structure has a determining role in the generation of patterns after bifurcation. As of today, the post-bifurcating patterns are obtained by solving the equilibrium equations for the specific loading condition of the problem. In this work, we make use of the symmetries of the structure by presenting a group-theoretic approach to develop a method capable of predicting the post-bifurcated patterns attainable by 2D architectured lattice materials.

Keywords: Architectured materials, pattern generation, bifurcation, symmetry groups

1 Introduction

Since the 1980s, extensive numerical, theoretical and experimental studies on hexagonal honeycombs under in-plane compression have shown that the structure can exhibit multiple post-buckling patterns, depending on the boundary conditions it is subject to.Furthermore, the symmetry of the structure plays a decisive role on the emergence of buckled patterns in its post-bifurcated configurations [1].

Findings from group [1] have determined that symmetry plays a decisive role in the emergence of these patterns. Therefore, group theory is used to determine the post-bifurcated paths of the material under compression, by helping solve the system's governing equations [2]. In this work, we present a new method which depends only on the symmetry of the structure to predict the patterns of post-bifurcated architectured materials.

2 Method

For regular hexagonal honeycombs, the bifurcation mechanisms can therefore be assessed by studying the symmetry of its representative surface element: $D_6 \ltimes (\mathbb{Z}_2 \times \mathbb{Z}_2)$ [3]. After computing the irreducible representations of this symmetry group, we determine its maximal isotropy subgroups, which are candidates for the symmetry groups of bifurcated solutions. To conclude on the existence of a solution, we use the Equivariant Branching Lemma (EBL) [4] on each of the candidates to conclude if the bifurcations can take place. Once the symmetries have been identified, we mesh our representative surface with beam elements and constrain the displacements of its nodes using the symmetries found with the EBL.

3 Results

The method was validated using the numerical and experimental results from the literature (see figure 2). We obtain the following :

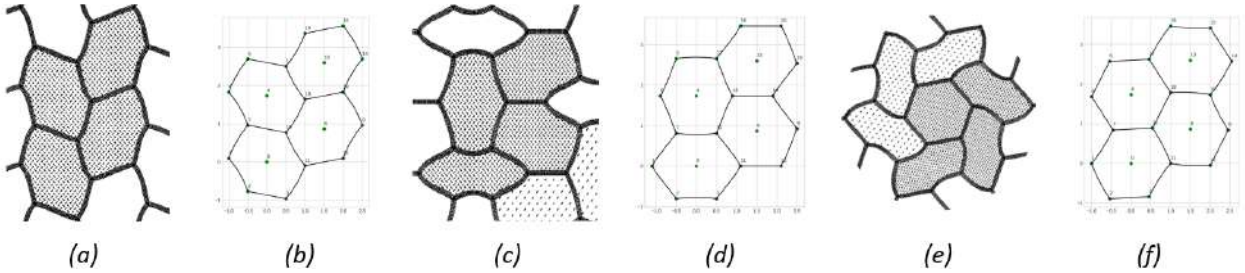


Figure 1: Results obtained using the method explained in the previous section. *(a) Mode I, (c) Mode II, (e) Mode III, from [1]. (b) Mode I, (d) Mode II, (f) Mode III, results obtained using our method.*

4 Conclusion

We have developed a method to predict the possible patterns of post-bifurcated honeycombs. So far the results we obtain are identical to those found experimentally, numerically and theoretically in the literature. This method being based on group theory, it can be extended to any other symmetry group.

5 Acknowledgements

This work was funded by Agence Nationale de la Recherche through the ANR MAX-OASIS project (Grant No. ANR-19-CE08-0005).

References

[1] Ohno, D. Okumura, and H. Noguchi, *Journal of the Mechanics and Physics of Solids*, vol. 50, no. 5, pp. 1125–1153, 2002.

[2] C. Combescure, P. Henry, R. S. Elliott, *International Journal of Solids and Structures*, Volumes 88–89, Pages 296-318, 2016.

[3] K. Ikeda and K. Murota, *Imperfect bifurcation in Structures and Materials*, 2002.

[4] M. Golubitsky, I. Stewart, and D. G. Schaeffer, *Singularities and Groups in Bifurcation Theory: Volume II*, 1988.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Beam lattice metamaterials with internal contact and instabilities

Martin Horák[*,†], **Emma La Malfa Ribolla**[‡] **and Milan Jirásek**[†]

[†] Faculty of Civil Engineering
Czech Technical University in Prague
Prague 6, Czech Republic
e-mail:{martin.horak, milan.jirasek}@fsv.cvut.cz

[‡] Department of Engineering
University of Palermo, Italy
e-mail: emma.lamalfaribolla@unipa.it

Abstract: Flexible and soft mechanical metamaterials with artificially designed microstructures have attracted attention due to their unusual and tunable properties with applications in, e.g., soft robotics and energy harvesting. Moreover, the interest in such materials has been increased hand in hand with the progress in additive manufacturing, enabling the fabrication of the designed microstructures.

The classical mechanical metamaterials include, e.g., auxetic (negative Poisson's ratio) metamaterials [1], metamaterials with vanishing shear modulus, and topological metamaterials [2]. Another exciting group of metamaterials consists of the so-called programmable materials whose properties can be switched by external stimuli. To achieve such a behavior, we propose an architected hexagonal lattice with an additional internal contact mechanism. Careful design and rearrangement of the underlying contact mechanism lead to tunable stiffness, which can be adapted to a specific application.

The design of the proposed metamaterial relies upon a robust and efficient computational tool. The development of such a tool is challenging mainly due to the internal contact and large deformations of the lattice with a possibility to develop instabilities. Therefore, the adopted computational method is based on the recently proposed geometrically exact beam element [3]. Moreover, the element formulation is extended to incorporate the contact internally, leading to a very efficient formulation.

Keywords: Metamaterial, Hexagonal Lattice, Internal Contact, Geometrically Nonlinear Beam Element

Acknowledgment: The authors gratefully acknowledge the financial support of the Czech Science Foundation, through the project No. 19-26143X.

References

[1] Lakes, R. Foam structures with a negative Poisson's ratio. *Science* (1987) **235**:1038–1041.

[2] Yu, X., Zhou, J., Liang, H., Jiang, Z. and Wu, L. Mechanical metamaterials associated with stiffness, rigidity and compressibility: A brief review. *Prog. Mater. Sci.* (2017) **94**:114–173.

[3] Jirásek, M., La Malfa Ribolla, E., Horák, M. Efficient geometrically nonlinear formulation of a beam element. *Submitted.*

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Pneumatic actuation of a square lattice metamaterial to control macroscopic stiffness

Faltus Ondřej[*†], Zeman Jan[*], Peerlings Ron[†], Jirásek Milan[*], Rokoš Ondřej[†], Horák Martin[*], and Doškář Martin[*]

[*] Department of Mechanics
Faculty of Civil Engineering, Czech Technical University in Prague
Prague, Czech Republic
e-mail: ondrej.faltus@cvut.cz

[†] Mechanics of Materials
Department of Mechanical Engineering, Eindhoven University of Technology
Eindhoven, The Netherlands

Abstract: Mechanical metamaterials feature an artificially designed microstructure resulting in specific macrostructural mechanical behavior [1]. Active metamaterials [2] can change their properties without change in geometry, for example, by pneumatic actuation [3, 4]. Pattern-forming metamaterials are two-dimensional polymer sheets that change their macroscopic properties due to internal instability [5, 6, 7]. We propose to unify these concepts in a two-dimensional square lattice metamaterial whose macroscopic stiffness under compression can be repeatedly tuned by pressure actuation. First, we test the idea and determine an expected range of the resulting stiffness using a microstructure in which the different wavelengths are predetermined by its initial geometry. We perform computational tests on a finite element RVE model and find the expected effect in line with our predictions. We then transition to a pneumatically actuated microstructure with switchable stiffness triggered by changing air pressure in the voids of the square lattice while still retaining the same initial geometry. Based on systematic computational testing, we find the concept feasible, yet still not entirely fulfilling the initial promise. Design drawbacks are identified, namely the presence of transversal material ligaments posing a problem to fully developing the desired pressurized shape. We develop more complicated microstructure designs to show how the concept could be improved.

Keywords: Mechanical Metamaterial, Pneumatic Actuation, Active Metamaterial, Switchable Stiffness

Acknowledgment: This work has been supported by the Czech Science Foundation, project no. GA19-26143X.

References

[1] Yu, X., Zhou, J., Liang, H., Jiang, Z., and Wu, L. (2018). Mechanical metamaterials associated with stiffness, rigidity and compressibility: A brief review. Progress in Materials Science, 94:114–173. doi:10.1016/j.pmatsci.2017.12.003

[2] Pope, S. A., and Laalej, H. (2014). A multi-layer active elastic metamaterial with tuneable and simultaneously negative mass and stiffness. Smart materials and structures,

23(7), 075020. doi:10.1088/0964-1726/23/7/075020

[3] Khodasevych, I., Rowe, W., and Mitchell, A. (2012). Reconfigurable fishnet metamaterial using pneumatic actuation. Progress in Electromagnetics Research B, 38:57–70. doi:10.2528/PIERB11102505

[4] Hedayati, R., and Lakshmanan, S. (2020). Pneumatically-actuated acoustic metamaterials based on Helmholtz resonators. Materials, 13(6), 1456. doi:10.3390/ma13061456

[5] S. D. Papka and S. Kyriakides. Biaxial crushing of honeycombs: Part I: Experiments. International Journal of Solids and Structures, 36(29):4367–4396, 1999. doi:10.1016/S0020-7683(98)00224-8.

[6] S. D. Papka and S. Kyriakides. In-plane biaxial crushing of honeycombs: Part II: Analysis. International Journal of Solids and Structures, 36(29):4397–4423, 1999. doi:10.1016/S0020-7683(98)00225-X.

[7] T. Mullin, S. Deschanel, K. Bertoldi, and M. C. Boyce. Pattern transformation triggered by deformation. Physical Review Letters, 99(8):084301, 8 2007. doi:10.1103/PhysRevLett.99.084301.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Projection-based model order reduction for creep behavior in prestressed concrete structures

Agouzal Eki[1,2,3], Argaud Jean-Philippe[1], Bergmann Michel[2,3], Ferté Guilhem[1], Taddei Tommaso[2,3]

[1] EDF Lab Paris-Saclay, EDF R&D
7 Boulevard Gaspard Monge
Palaiseau, France

[2] INRIA, Inria Bordeaux Sud-Ouest, Team MEMPHIS
Université de Bordeaux
Talence, France

[3] Institut de Mathématiques de Bordeaux (IMB), UMR 5251
Université de Bordeaux
Talence, France

Abstract: We propose a projection-based model order reduction procedure for the aging of large prestressed concrete structures. Our work is motivated by applications in the nuclear industry, particularly in the analysis of containment buildings. Such numerical simulations involve a multi-modeling approach: a three-dimensional nonlinear rheological model is used for the concrete, and prestressing cables are described by a one-dimensional elastic behavior. We develop an adaptive algorithm based on a POD-Greedy strategy driven by a cost-efficient error indicator. We develop an hyper-reduction strategy using an element-wise empirical quadrature in order to speed-up online assembly costs. We provide numerical results on a stantard section of a double-walled containment building.

Keywords: parametrized partial differential equations, model order reduction, hyperreduction, creep, prestressed concrete

1 Context

Numerical simulations provide a key decision-making tool for engineers in the scope of industrial projects. Within the framework of engineering studies in the nuclear industry, the ageing of containment buildings is a key research topic. The behavior of heterogeneous and porous concrete is governed by complex thermo-activated phenomena. Since the decoupling of the physical mechanisms involved is valid for large structures under normal operating loads, a weak thermo-hydro-mechanical (THM [1]) coupling procedure is considered to model the deferred deformations within the material. However, engineers might need to repeat numerical simulations for slightly different configurations in order to assess the mechanical state of the material. The high-computational costs of the high-fidelity (HF) procedure is a barrier to using efficiently parametric (many-queery) studies. We provide an intrusive parametric model order reduction (pMOR) for those prestressed concrete structure to circumvent this issue.

2 Projection-based ROM for nonlinear mechanics

2.1 HF prestressed concrete modeling

We consider small-strain small displacements problems, and we consider a three-dimensional domain divided in one subdomain for the concrete and another for the steel cables. We deal with a multi-modeling framework, where a non-linear model (rheological creep model) is adopted for the concrete, and the prestressing cables are described by a one-dimensional linear elastic behavior modelisation. A kinematic linkage is performed in order to connect the concrete nodes and the steel nodes: a point within the steel and its coincident point in the concrete are assumed to have the same displacement.

2.2 Projection-based ROM and adaptive strategy

We implement an hyper-reduced ROM based on a qualified and broadly-used industrial grade finite element solver for structural mechanics (code_aster [2]). Our numerical strategy relies on a Galerkin projection method. The reduced order basis computed through Proper Orthgonal Decomposition (POD [3]) thanks to previsously computed HF snapshots. The non-linearity of the operator entails that the computational cost of the ROM assembly scales with the size of the HF model. We develop an hyper-reduction strategy based on empirical quadrature (EQ) to bypass this computational bottleneck: our approach relies on the construction of a reduced mesh (Figure (1)) to speed up online assembly costs of the ROM. We choose to use a re-weighting of the mesh elements [5], thanks to the Energy-Conserving Sampling and Weighting method (ECSW [6]).

(a) HF mesh

(b) Example of a hyper-reduced mesh

Figure 1: Examples of meshes of standard section: (a) HF case; (b) reduced case

We develop an adaptive algorithm, based on a POD-Greedy procedure which iteratively explores the parameter domain to identify poorly approximated configurations and enrich the ROM in order to better approximate the parametric manifold. Moreover, we introduce a cost-efficient error indicator correlated to the approximation error, which can be thus used to drive the Greedy procedure.

3 Conclusions and Perspectives

Our first numerical results display an efficiency of the model reduction process implemented. The model reduction and the hyper-reduction procedure used brings interesting results on speedups, even on a relatively coarse mesh, while keeping good approximation errors on the variables of interest. The work still needs to be extended by testing more parametric problems, and on larger mesh sizes, in order to evaluate the performance of our reduction methodology. A prospect of this work is the application of this approach to the design of a surrogate model for inverse problems.

4 Acknowledgements

This work was partly funded by ANRT (French National Association for Research and Technology) and Electricité de France (EDF).

References

[1] Bouhjiti D. Analyse Probabiliste de La Fissuration et Du Confinement Des Grands Ouvrages En Béton Armé et Précontraint. Université Grenoble Alpes; 2018.

[2] Electricité de France. Finite element code_aster, Analysis of Structures and Thermomechanics for Studies and Research. Open source on www.code-aster.org; 1989-2022

[3] Berkooz G, Holmes P, Lumley JL. The proper orthogonal decomposition in the analysis of turbulent flows. Annual review of fluid mechanics. 1993;25(1):539–575.

[4] Sirovich L. Turbulence and the dynamics of coherent structures. I. Coherent structures. Quarterly of applied mathematics. 1987;45(3):561–571.

[5] Iollo A, Sambataro G, Taddei T. An adaptive projection-based model reduction method for nonlinear mechanics with internal variables: Application to thermo-hydro-mechanical systems. International Journal for Numerical Methods in Engineering. 2022;123(12):2894–2918.

[6] Farhat C, Avery P, Chapman T, Cortial J. Dimensional reduction of nonlinear finite element dynamic models with finite rotations and energy-based mesh sampling and weighting for computational efficiency. International Journal for Numerical Methods in Engineering. 2014;98(9):625–662.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Online adaptation of the parametric reduced order model of a gas bearings supported rotor

Dimitri Goutaudier*†, Fabio Nobile* and Jürg Schiffmann*

*École Polytechnique Fédérale de Lausanne, Switzerland
†e-mail: dimitri.goutaudier@gmail.com

Abstract: The hybrid twin paradigm, which involves using physics-based surrogate models that incorporate sensor data to improve predictions, is gaining increasing attention in engineering applications [2]. In this study, we present the first steps towards developing a hybrid twin of a gas bearings supported rotor. Unlike traditional ball bearings that use mechanical contact, the rotor is here supported by an aerodynamic force which is generated by pressurized gas flowing through the bearing [1]. This technology requires extremely high rotation speeds with tight clearances, making model-assisted operations of such dynamical systems very challenging. We propose a projection-based parametric Reduced Order Model (pROM) that can perform fast and physically interpretable simulations of the system. The pROM is constructed by projecting the governing equations onto a low-dimensional subspace spanned by a reduced basis computed with the Proper Orthogonal Decomposition (POD) [3]. The nonlinear terms are handled with the Discrete Empirical Interpolation Method (DEIM), which is a sparse sampling technique [4]. We then explore different approaches for adapting online the pROM for changes in the system's parameters, including reduced bases interpolation techniques [5] and low-rank updates [6]. Interpolation techniques allow to compute new reduced bases from the available ones, while low-rank updating techniques use synthetic or measured data to update the reduced bases. The developed pROM is then applied to a shock identification problem. In some applications, a turbomachinery may indeed experience sudden dynamical loadings, which can perturb the rotor orbits and ultimately lead to damages. We then propose an inverse method to identify the shock parameters from measurements of the rotor orbits in the two bearings. The proposed approach shows great potential for model-assisted monitoring and control of the rotor. However, further research is needed to address the real-time constraint for industrial applications.

Keywords: parametric Model Order Reduction (pMOR), reduced basis adaptation, parameters identification, gas bearings, dynamical systems

References

[1] Gu L, Guenat E, Schiffmann J. (2020). A review of grooved dynamic gas bearings. Applied Mechanics Reviews, 72(1).

[2] Chinesta F, Cueto E, Abisset-Chavanne E, Duval JL, Khaldi FE. (2020). Virtual, digital and hybrid twins: a new paradigm in data-based engineering and engineered data. Archives of computational methods in engineering, 27(1), 105-134.

[3] Benner P, Gugercin S, Willcox K. (2015). A survey of projection-based model reduction methods for parametric dynamical systems. SIAM review, 57(4), 483-531.

[4] Chaturantabut S, Sorensen DC. (2010). Nonlinear model reduction via discrete empirical interpolation. SIAM Journal on Scientific Computing, 32(5), 2737-2764.

[5] Amsallem D, Farhat C. (2008). Interpolation method for adapting reduced-order models and application to aeroelasticity. AIAA journal, 46(7), 1803-1813.

[6] Peherstorfer B, Willcox K. (2015). Online adaptive model reduction for nonlinear systems via low-rank updates. SIAM Journal on Scientific Computing, 37(4), A2123-A2150.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A grey-box framework for flaw localization exploiting Ultrasonic Guided Waves

Paul Sieber*, Sergio Nicoli*, Konstantinos Agathos†, Pawel Kudela‡, Wieslaw Ostachowicz‡ and Eleni Chatzi*

* Institute of Structural Engineering (IBK)
Eidgenössische Technische Hochschule Zürich (ETH Zurich)
Zurich, Switzerland
e-mail: {sieber, nicoli, chatzi}@ibk.baug.ethz.ch

† University of Exeter,
Exeter, UK
e-mail: k.agathos@exeter.ac.uk

‡ Institute of Fluid-Flow Machinery
Polish Academy of Sciences
Gdansk, Poland
e-mail: {pawel.kudela, wieslaw.ostachowicz}@imp.gda.pl

Abstract: Ultrasonic Guided Waves (UGWs) boast the ability to detect small defects due to their short wavelength. This enables flaw detection at an early stage. In order to bestow a Structural Health Monitoring (SHM) system with flaw localization potential it is advantageous to fuse measured UGW data with physics-based models. These models can accomplish a forward simulation of the UGW behaviour. As the forward simulation of UGW propagation requires fine discretization in space and time, such simulations are typically computationally prohibitive. This points to the need for efficient forward simulations, which can feed inverse schemes that require multiple forward simulations.

This contribution uses the Spectral Element Method (SEM) in the time domain and combines it with an efficient, mesh-independent feature to introduce flaws to the structure. Next, two different inverse algorithms are tested in terms of their potential for localization; the first scheme relies on Radial Basis Functions (RBFs) and the latter on Covariance Matrix Adaption Evolution Strategies (CMA-ES).

The damage detection scheme is numerically illustrated on a modelled aluminium plate. Based on this illustration, the efficacy of the SEM scheme for defect detection will be investigated. Furthermore, advantages and disadvantages of the tested inverse solvers will be highlighted.

Keywords: Ultrasonic guided waves (UGW), Structural health monitoring (SHM), Damage detection, Defect Localization

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Data-Driven Model-Order Reduction of a Nonlinear Finite-Element Model based on DIC Measurements

F. N. Kristiansen[1,a], **A. L. Klausen**[1,b], **G. Miraglia**[2,a], **G. Abbiati**[1,c]

[1]Dep. of Civil and Arch. Eng., Aarhus University, Denmark
e-mail: [1,a]au588382@post.au.dk, [1,c]abbiati@cae.au.dk

[2]Dep. of Struct., Geotech. and Building Eng., Polytechnic of Turin, Italy
e-mail: [2,a]gaetano.miraglia@polito.it

Abstract: This extended abstract demonstrates a projection-based model-order reduction (MOR) method that utilizes digital image correlation (DIC) data to construct the reduction basis. The methodology is applied to reduce the computational cost associated with the nonlinear static analysis of a masonry wall.

Keywords: Model order reduction, digital image correlation, nonlinear finite-element analysis

1 Methodology

In projection-based MOR, the displacement vector of the FE model is projected into a manifold of reduced rank $\mathbf{u} = \mathbf{V}\hat{\mathbf{u}}$ where $\hat{\mathbf{u}}$ is a reduced-order displacement vector. In this work, $\mathbf{V}$ is computed from experimental data using proper orthogonal decomposition.

$$\mathbf{U} = \begin{bmatrix}\mathbf{u}_1 \dots \mathbf{u}_l\end{bmatrix} = \mathbf{\Phi}\mathbf{\Sigma}\mathbf{\Lambda}^T \tag{1}$$

where $\mathbf{U}$ is a collection of snapshots of the displacement field $\mathbf{u}$ of the structure measured on a physical experiment, $\mathbf{\Phi}$ is the matrix of proper orthogonal modes (POMs), $\mathbf{\Sigma}$ is the matrix of singular values and $\mathbf{\Lambda}$ is the matrix of time modulating functions. The MOR matrix is obtained as $\mathbf{V} = \mathbf{\Phi}_{1:m}$, where m is the number of retained POM [1].

2 Application

The application example builds upon the masonry facade described in [2] and depicted in Figure 1a. The wall was subjected to seismic excitation using hybrid testing. DIC was used

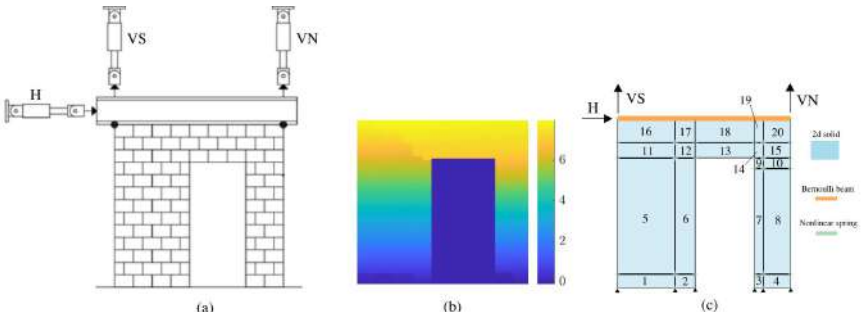


Figure 1: a) Physical model [2], b) DIC snapshot of horizontal displacement field and c) numerical model

to acqurie the displacement field during the test. In a FE macro-model linear elastic 2d solid

elements are coupled with nonlinear springs that simulate crack opening [3] as presented in Figure 1c. A sigmoid function modulates Young modulus of solid 2d element to mimic stiffness degradation. A major issue in using DIC data to construct the MOR is that the FE model is not capable of reproducing the exact crack pattern observed during the experiment. Specifically, a 2d solid element might cross a crack. If such a 2d solid element would be enforced to follow such a deformational shape, the corresponding restoring force would be unrealistically large. In order to prevent this to happen, the following extrapolation is adopted; i) elimination of image points over cracks using strain data, ii) density-based spatial clustering of the data points in (x, y, u)-space and iii) nodal displacement extrapolation on the largest point cluster.

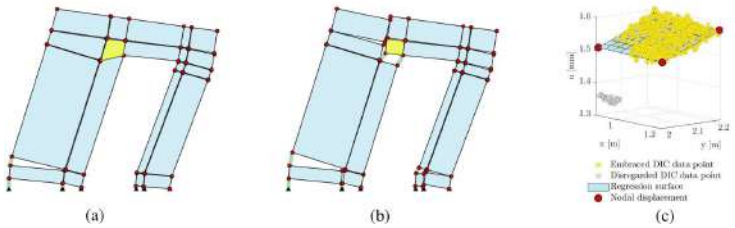


Figure 2: Node displacement tracking in DIC with a) direct approach and b) cluster extrapolation approach. c) presents the cluster extrapolation approach applied on element 12

Figure 2 presents node displacement tracking in DIC for the proposed cluster extrapolation approach compared with a more direct approach, where the nearest DIC data point within the connected 2d solid is tracked. After MOR, the computational cost for a nonlinear static analysis of the FE model requires 24 sec on a standard laptop, that is, 47 % less than the full-order model. Figure 3 compare the experimental response of the wall to the numerical one computed using the calibrated ROM. As one can see, the ROM response represents fairly well the original wall.

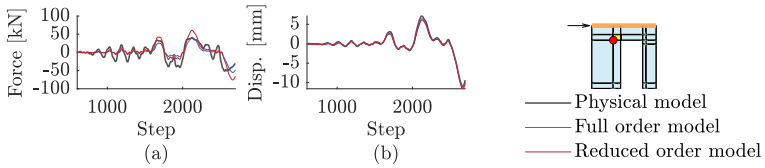


Figure 3: a) Horizontal force in actuator H and b) horizontal displacement in node 45

3 Conclusions

The proposed data-driven MOR speeds up the simulation by about 47%. Projection-based MOR seems to be promising for fusing data and first-principle models for high-fidelity yet computationally cheap numerical simulations.

References

[1] Farhat et al., Int. Journal for Numerical Methods in Eng., 102:1077-1110, 2015.

[2] Miraglia et al., Earthquake Eng. & Struct. Dyn., 49(8):737-753, 2020.

[3] McGarry, et al., Journal of the Mechanics and Physics of Solids, 63:336–362, 2014

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical techniques towards competitive partitioned solution strategies for thermomechanical contact problems

António M. Couto Carneiro[*†], José L. P. Vila-Chã[*†], Rodrigo Pinto Carvalho[†], Bernardo P. Ferreira[‡], Francisco M. Andrade Pires[*†]

[*] Department of Mechanical Engineering (DEMec)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: {amcc,jvc,fpires}@fe.up.pt

[†] Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI)
Porto, Portugal
e-mail: rpcarvalho@inegi.up.pt

[‡] School of Engineering, Brown University,
Providence, USA
e-mail: bernardo_ferreira@brown.edu

In the current scientific landscape, the challenges associated with the simulation of thermomechanical contact are twofold. First, robust discretisation techniques are mandatory to obtain an accurate and stable approximation of the interface fields [1]. Second, an efficient solution to the coupled problem is most desirable. Monolithic techniques solve the coupled problem simultaneously. Besides the inherent temporal stability, they ensure excellent performance when combined with well-designed linear solver technology. Partitioned techniques solve the fields separately and are equipped with communication channels to realise the coupling. In particular, strong coupling techniques are originally built on top of fixed-point iterations to replicate the fully-coupled solution. These schemes are much simpler to implement and maintain, but may face convergence issues for strong physical coupling, which can be minimised with acceleration techniques [2].

Despite the maturity of acceleration and coupling techniques in other multi-physics fields, their application in thermomechanical contact problems is still very scarce. This work extends a previous contribution by the authors with a benchmark of partitioned coupling techniques focusing on thermomechanical contact [3]. Different aspects of the phenomenon are investigated using dedicated examples, with varying coupling degrees. The results demonstrate significant performance gains, levelling the competition with monolithic strategies.

Keywords: Thermomechanical Contact, Acceleration Techniques, Partitioned Solution

References

[1] Seitz, Alexander, Wolfgang A. Wall, and Alexander Popp. “A Computational Approach for Thermo-Elasto-Plastic Frictional Contact Based on a Monolithic Formulation Using Non-Smooth Nonlinear Complementarity Functions.” *Advanced Modeling and Simulation in Engineering Sciences* 5, no. 1 (March 2, 2018): 5.

[2] Erbts, Patrick, and Alexander Düster, Accelerated Staggered Coupling Schemes for Problems of Thermoelasticity at Finite Strains, *Computers & Mathematics with Applications* 64, no. 8 (October 1, 2012): 2408–30.

[3] Vila-Chã, José L. P., António M. Couto Carneiro, Bernardo P. Ferreira, and F. M. Andrade Pires. “A Numerical Assessment of Partitioned Implicit Methods for Thermomechanical Problems.” *Computers & Structures* 277–278 (March 1, 2023): 106969.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Fast Boundary Element Methods for fault mechanics and earthquake control

Laura Bagur[*], Stéphanie Chaillat[*], Jean-François Semblat[†], Ioannis Stefanou[‡] and Pierre Romanet[II]

[*] POEMS Laboratory
CNRS, Inria, ENSTA Paris, Institut Polytechnique de Paris
Palaiseau, France
e-mail: (laura.bagur,stephanie.chaillat)@ensta-paris.fr

[†] IMSIA Laboratory
CEA, CNRS, EDF, ENSTA Paris, Institut Polytechnique de Paris
Palaiseau, France
e-mail: jean-francois.semblat@ensta-paris.fr

[‡] Institut de Recherche en Génie Civil et Mécanique
(UMR CNRS 6183) Ecole Centrale de Nantes
Nantes, France
e-mail: ioannis.stefanou@ec-nantes.fr

[II] Earthquake and Tsunami Research Division
NIED
Tsukuba, Ibaraki, Japan
romanet@bosai.go.jp

Abstract: This work focuses on the simulation of sequences of seismic and aseismic slip events using Fast boundary element methods (BEMs). An algorithm based on FFT-accelerated BEMs is first considered, validated and results are shown for a basic problem in crustal faulting. These developments target the formulation of efficient computational tools for studying fluid-injection-induced seismicity and to investigate its possible mitigation numerically. A first multi-physics case using accelerated BEMs to solve the previous crustal faulting problem with fluid injection is considered.

Keywords: Fast Boundary Element Methods (Fast BEMs), Fault mechanics, Seismic control, Fluid-injection-induced seismicity.

1 Motivations : Assessment of earthquake control strategies by fluid injection

Earthquakes due to either natural or anthropogenic sources cause important human and material damage. In both cases, the presence of pore fluid influence the triggering of seismic instabilities. Preliminary results, done in the context of the European Research Council CoQuake's project (`www.coquake.eu`), show that the earthquake instability could be avoided by active control of the fluid pressure [1].
In this contribution, we propose to study the ability of Fast Boundary Element Methods (Fast BEMs) [2] to provide a multi-physic large-scale robust model required for modeling earthquake processes, human-induced seismicity and their control.

2 Existing methods for fault mechanics

The main methods used for numerical modeling of earthquake ruptures at a planar interface between two elastic half-spaces are spectral BEMs as in [3]. As a first step, we consider this method for a simple problem in crustal faulting. Let us consider a 1D planar vertical strike-slip fault, embedded in a 2D homogeneous, linear elastic infinite space Figure 1. The antiplane shear movement assumed in the x direction leads to a displacement on either side of the fault independent of the x coordinate. The fault is obeying an empirical rate-and-state friction law. BEMs applied to the local balance law combined with Hooke's constitutive law, leads to a relation between the jump in displacement denoted δ across the fault and the shear stress f due to quasi-static deformation:

$$f(z,t) = \frac{\mu}{2\pi} \int_{\Gamma} \frac{1}{z - z'} \frac{\partial \delta}{\partial z'}(z',t) dz' \tag{1}$$

where, Γ corresponds to the fault interface, and μ is the shear modulus. The calculation of f can be easily speed-up in the Fourier space:

$$F(\xi,t) = -\frac{\mu|k|}{2} D(\xi,t), \;\; k = 2\pi\xi \tag{2}$$

This technique is only valid for planar faults. We also propose an alternative speed-up technique using BEMs accelerated with Hierarchical Matrices, which enables to solve more realistic problems in crustal faulting. To solve this problem, different adaptive time stepping algorithms inspired from the literature ([3], [4], and [5]) are tested in order to take into account both small and large time scales with the correct resolution in time. We validate the implemented methods considering the case where on-fault unknows are constant in time, which leads to have the unknowns equal to their initial values. Figure 2 shows sequences of seismic and aseismic phases (which last about 108 s and 84 yrs in average respectively).

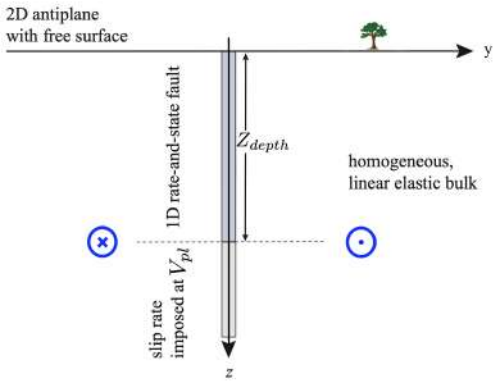


Figure 1: Representation of the 1D anti-plane problem

3 Incorporating hydro-mechanical couplings

Then, poroelastodynamic effects are considered. To this aim, a dimensional analysis of generic poroelastodynamic equations [6] is performed. It allows determining which of the

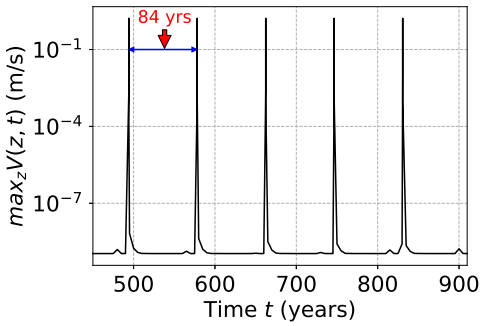


Figure 2: Maximal slip rate at depth evolution with respect to time

poroelastodynamics effects are predominant depending on the observation time of the fault. The obtained equations corroborate and justify simplified multiphysics models from the literature, for example [7]. A first multi-physics test using Fast BEMs to solve a simplified crustal faulting problem with fluid injection is considered.

4 Perspectives

The objective of this project is to provide a viable efficient tool to explore the advantages and limitations of novel strategies of earthquake control using fluid injection to drive the fault from an unstable state of high potential energy to a stable state of lower potential energy. Ongoing work concerns the extension of Fast Boundary Element methods to fault mechanic problems incorporating the effect of fluid injection of the on-fault behaviour

5 Acknowledgements

This work is supported by a Contrat Doctoral Spécifique Normalien (CDSN) and forms part of the ERC project CoQuake (Controlling earthQuakes, www.coquake.eu), funded by the European Research Council (ERC, `https://erc.europa.eu/`) under the European Union's Horizon 2020 research and innovation program (Grant agreement n°757848 CoQuake).

References

[1] I. Stefanou. Controlling Anthropogenic and Natural Seismicity: Insights From Active Stabilization of the Spring-Slider Model, Journal of Geophysical Research: Solid Earth, 8786-8802, 2019.

[2] S. Chaillat, M. Bonnet. Recent advances on the fast multipole accelerated boundary element method for 3D time-harmonic elastodynamics, Wave Motion, 1090-1104, 2013.

[3] N. Lapusta, J. Rice and al. Elastodynamic analysis for slow tectonic loading with spontaneous rupture episodes on faults with rate- and state-dependent friction, Journal of Geophysical Research: Solid Earth, 23765-23789, 2000.

[4] P. Romanet, S. Ozawa. *Fully Dynamic Earthquake Cycle Simulations on a Nonplanar Fault Using the Spectral Boundary Integral Element Method (sBIEM)*, Bulletin of the Seismological Society of America, 2021.

[5] S. Ozawa, A. Ida, T. Hoshino, R. Ando *Large-scale earthquake sequence simulations on 3D nonplanar faults using the boundary element method accelerated by lattice H-matrices.*, Geophysical Journal International, 232(3), 1471-1481., 2022

[6] M. Schanz. Poroelastodynamics: Linear Models, Analytical Solutions, and Numerical Methods., Applied Mechanics Reviews, 62(3)., 2009.

[7] E. R. Heimisson, J. Rudnicki, N. Lapusta. Dilatancy and Compaction of a Rate-and-State Fault in a Poroelastic Medium: Linearized Stability Analysis., Journal of Geophysical Research: Solid Earth, 126(8), 2021

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Contact-dominated architected materials

Konstantinos Karapiperis[†] **and Dennis M. Kochmann**[†]

[†] Mechanics & Materials Lab, Dept. of Mechanical and Process Engineering, ETH Zurich, Switzerland
e-mail: kkarapiperis@ethz.ch, dmk@ethz.ch

Abstract: The design of architected materials has succesfully harnessed concepts such as hierarchy, instability, and defects, in order to produce enhanced and tunable mechanical behavior. On the other hand, self-contact and friction has only recently been explored as a mechanism for improving material properties [1-3]. In this work, we demonstrate how manipulating frictional contact in different families of truss- and fiber-based materials (e.g. interpenetrating lattices, woven lattices, entangled materials) allows for controlled stiffening and tunable energy absorption. To efficiently explore these mechanisms, we develop a regularized variational beam contact theory able to capture challenging contact scenaria in a unified formulation, and can handle arbitrary friction laws. We complement our simulations with experiments of additively manufactured materials. This methodology paves the way for optimization over this new dimension of the design space of architected materials.

Keywords: Architected materials, Woven lattices, Truss lattices, Entangled materials, Contact mechanics

References

[1] Moestopo, W., Mateos, Arturo J. and Fuller, Ritchie M. and Greer, Julia R. and Portela, Carlos M. (2020). Pushing and Pulling on Ropes: Hierarchical Woven Materials. *Advanced Science*, 7(20), 1-11.

[2] White, B. C., Garland, A., Alberdi, R., and Boyce, B. L. (2021). Interpenetrating lattices with enhanced mechanical functionality. *Additive Manufacturing*, 38, 101741.

[3] Karapiperis, K. and Monfared, S. and Macedo, R and Richardson, S and Andrade, J. E (2022). Stress transmision in entangled granular structures *Granular Matter*, 24(3).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Isogeometric contact within machining applications

Eugen Salzmann[*], Florian Zwicke[†] and Stefanie Elgeti[†]

[*] Chair for Computational Analysis of Technical Systems (CATS)
RWTH Aachen
Aachen, Germany
e-mail: salzmann@cats.rwth-aachen.de

[†] Institute of Lightweight Design and Structural Biomechanics (ILSB)
TU Wien
Vienna, Austria
e-mail: {zwicke, elgeti}@ilsb.tuwien.ac.at

Abstract: Simulations for predicting critical process variables in machining applications have been carried out for years. One important simulation-based analysis class in this context is the Finite Element Method (FEM) [1]. It is challenging to model the process with FEM as the metal is subjected to extensive deformation at high strain rates and temperatures. This large deformation is primarily irreversible and requires a plastic material model. The so-called orthogonal cutting process is a good abstraction of machining applications, where only a 2D representation is considered. It involves a tool cutting through a workpiece, forming chips. The shape of these chips is a crucial validation criterion for the accuracy of the simulation. One way to improve the representation of geometries in FEM simulations is to utilize Isogeometric Analysis (IGA), where the classical Lagrangian basis functions are replaced by the basis of Non-Uniform Rational B-Splines (NURBS). As these splines are commonly used for the representation of geometries in CAD models, IGA bridges the analysis with the initial design geometry [2].

One crucial detail to model is the contact between the tool and the work piece. In this work we model the tool as a rigid B-Spline and employ a penalty contact formulation. Our focus is to investigate the influence of employing Isogeometric Analysis for the chip forming process and the resulting chips. Furthermore, we compare the results to a classical FEM approach.

Keywords: FEM, IGA, machining, computational contact

References

[1] Zabel A. Prozesssimulation in der Zerspanung: Modellierung von Dreh- und Fräsprozessen. Habilitation TU Dortmund; 2010.

[2] Hughes TJR, Cottrell JA, Bazilevs Y. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. Computer methods in applied mechanics and engineering 194: 4135-4195

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Constriction resistance of rough surfaces in contact

Paul Beguin, Vladislav A. Yastrebov

Mines Paris, PSL university, Centre des matériaux, CNRS UMR 7633, Evry, France
e-mails: paul.beguin@minesparis.psl.eu, vladislav.yastrebov@minesparis.psl.eu

Abstract: We study the thermal and electric resistance of individual contact clusters of complex shapes. Notably, we study how the connectedness of the spot and its geometrical compactness affect its conductivity. Further, we extend our study to contact zones made of many spots with and without oxide layers. This study was carried out using the fast boundary element method based on hierarchical matrices. Details of its implementation and a comparison with the finite element method are provided.

Keywords: Contact, roughness, electrical resistance, BEM, oxides

1 Introduction

Most engineering and natural systems involving contact between parts operate outside thermodynamic equilibrium and often involve thermal fluxes. Internal combustion engines (vehicles and aircrafts) and sliding of faults in the Earth's crust are two remarkable examples of relevant systems. The conductivity of contact interfaces is strongly dependent on the roughness of contacting solids, interfacial fluid and mechanical loads. The main thermal exchange between rough surfaces happens through intimate contact spots (true contact area). The thermal and also electric conductivity through such spots depend not only on the true contact area fraction but also on its morphology. The two of them evolve under the external load. Holm [1] and Greenwood [2] were among the first who realized the origin of the contact resitance and suggested simple models based on a set of interacting circular contact spots representing true contact area. However, at higher loads, the true contact area cannot be represented by a set of circular or elliptic spots but rather by complex not simply connected clusters [3] which represent the topic of this study. Furthermore, the morphology of contact clusters and the true contact area could be affected by thermal, chemical and metallurgical effects. Especially, formation of weakly conducting or insulating oxide layers strongly affect electrical resistance of contact interfaces.

1.1 Methods

To conduct the study on conductivity of contact spots of complex shape and their agglomerates Figs. 1,2, we implemented a fast boundary element method (fast-BEM) based on hierarchical matrices [4]. Such a method allows to overcome the main drawback of the classical BEM: storage and resolution of full matrices, which used to be a bottle neck of the method compared to the classical FEM. The problem of conductivity in contact interface reduces to the following integral equation

$$u(\boldsymbol{x}) = \int_{\partial\Omega_c} j_n(\boldsymbol{y}) G(\boldsymbol{x}, \boldsymbol{y}) dS \tag{1}$$

which should be solved for all contact clusters $\partial\Omega_c$ with u being the potential/temperature and j_n being the normal flux, $G(\boldsymbol{x}, \boldsymbol{y})$ is the Green function. This problem formulated for half-spaces is well adapted for the BEM, whose implementation will be presented in detail. Apart from simplified model shapes, we also study shapes resulting from contact simulations based on a spectral method. We demonstrate how the BEM and spectral method could operate efficiently together to solve weakly coupled multiphysical problems.

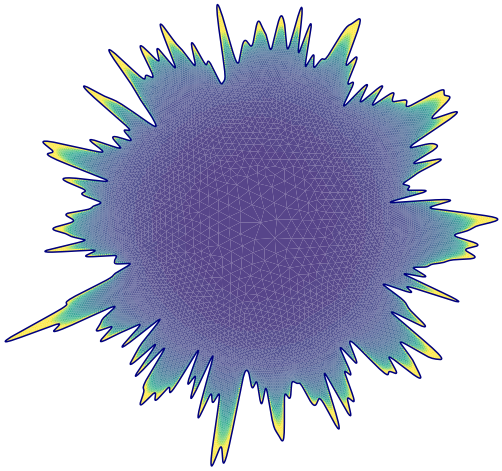


Figure 1: Simulated normal flux through a contact spot with random self-affine boundary

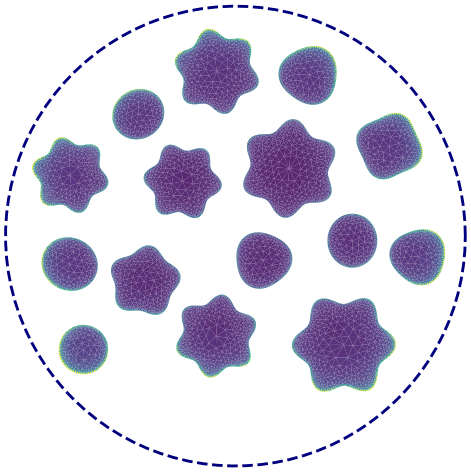


Figure 2: Simulated normal flux throug a multi-spot contact area

2 Results & Discussion

Several novel results on the conductivity of complex shapes were obtained thanks to the powerful fast-BEM, notably we established a relationship between fractal dimension and spectral breadth of a contact spot and its conductivity. For the multi-spot configuration we established limits of applicability of the Greenwood's model [2]. Finally, a method to take into account effect of oxide layers was established for different types of oxide.

References

[1] Holm, R. (1957). Electric contacts: theory and application. Springer.

[2] Greenwood, J.A. (1966). Constriction resistance and the real area of contact. British Journal of Applied Physics, 17(12):1621.

[3] Yastrebov, V. A., Anciaux, G., & Molinari, J. F. (2015). From infinitesimal to full contact between rough surfaces: evolution of the contact area. IJSS 52, 83-102.

[4] Chaillat, S., Desiderio, L. & Ciarlet, P. (2017). Theory and implementation of H-matrix based iterative and direct solvers for Helmholtz and elastodynamic oscillatory kernels. Journal of Computational physics, 351:165-186.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Non-linear Elasticity and Contact of Zinc-Phosphate Tribofilms

Lucas Frérot*, Lars Pastewka*

* Institut für Mikrosystemtechnik (IMTEK)
Albert-Ludwigs-Universität
Freiburg, Germany
e-mail: lucas.frerot@imtek.uni-freiburg.de

Abstract: Among the many applications of phosphate glasses, the tribologist is perhaps most familiar with zinc-phosphate tribofilms that form on steel surfaces as a result of ZDDP decomposition in high-temperature and high-friction environments such as car engines. Due to the decomposition process, surface roughness and high contact pressures, these tribofilms are chemically heterogeneous and have nonlinear elastic response, making modeling tribological properties a challenge. Here we present a framework combining molecular dynamics and volume integral equations to simulate the behavior in contact between a heterogeneous, nonlinear zinc-phosphate tribofilm and a rough surface. We analyze how its response deviates from the common assumption of homogeneous, linear elasticity used in rough-surface contact.

Keywords: zinc-phosphate glass; tribofilm; contact; rough surface; nonlinear elasticity

1 Introduction

Due to a wide range of glass-forming compositions, phosphate-based glasses enjoy applications in, among others, optics, bone repair, seals, and tribology. In the latter domain, they are commonly encountered as a product of the decomposition of zinc dialkyldithiophosphates (ZDDP), a family of additives used to reduce friction and wear. Thanks to a shear-stress assisted reaction, ZDDP decomposes into a protective tribofilm of zinc-phosphate glass that binds to steel surfaces in zones where the friction is most intense, thus protecting areas most likely to wear out. Once deposited, however, the balance between film growth and film destruction is poorly understood. In order to study and make predictions on the wear properties of these tribofilms, one needs models of its mechanical response in a realistic tribological interface. Composition heterogeneity (*i.e.* ortho- *vs.* poly-phosphate), pressure-dependent elasticity and surface roughness are key points that should be accounted for in the quantification of the wear response.

We consider these effects on a tribological contact with molecular models to evaluate the constitutive response and incorporate the identified mechanical behavior in a continuum approach for rough contact with nonlinear elastic, heterogeneous materials. Due to the fractal nature of rough surfaces, a Fourier-based volume integral equation approach is used. We will describe how the homogeneous Green's functions can be used in a heterogeneous setting appropriate for the modeling of realistic tribofilms.

2 Molecular model

To determine the mechanical properties of zinc-phosphate samples with varying composition and pressure, we use molecular dynamics simulations. Tischendorf et al. [1] have developed an approach based on the Lennard-Jones potential for pair interactions, a harmonic potential to enforce molecular geometry of phosphate chains and Coulomb interactions, with coefficients fitted to experimental zinc-phosphate structure characterization. While the simplicity of this modeling approach makes it attractive to homogenize elastic properties on large systems, these properties need to be independently validated. We therefore also use a density-functional tight-binding approach, where the force-field is derived from first principles. We find the results consistent with the Tischendorf et al. [1] force-field. We will briefly present constitutive laws as a function of chemical composition (*i.e.* phosphate chain length) and pressures up to 40 GPa, and show how they can be used in a continuum setting.

3 Rough contacts

Realistic rough surfaces being rough on a wide range of length-scales, numerical methods that can be used for simulations have to handle very large discretization requirements. This is the reason why Fourier-based boundary and volume integral methods [2] have become ubiquitous for rough surface contact simulations. However, they rely on the knowledge of Green's functions often derived for homogeneous, linear elastic media, or for particular, restricted cases, such as layered elastic [3], and are not directly applicable to materials where elastic properties may be dependent on position and pressure. Thanks to Eshelby's equivalent inclusion principle, which lets one replace the effect of heterogeneous elastic properties with a distribution of volumetric eigenstrains, one can use the homogeneous volumetric Green's functions [2] to solve the heterogeneous problem. We present in this work the derivation of the method in the Fourier domain and how it is used for high-performance solving of the rough, heterogeneous, non-linear contact problem.

4 Acknowledgments

The financial support of DFG grant #461911253 (AWEARNESS) is acknowledged.

References

[1] B. C Tischendorf, T. M Alam, R. T Cygan, and J. U Otaigbe. The structure and properties of binary zinc phosphate glasses studied by molecular dynamics simulations. 316(2):261–272. ISSN 0022-3093. doi: 10/ch66z2.

[2] Lucas Frérot, Marc Bonnet, Jean-François Molinari, and Guillaume Anciaux. A Fourier-accelerated volume integral method for elastoplastic contact. 351:951–976. ISSN 0045-7825. doi: 10.1016/j.cma.2019.04.006.

[3] Qiang Li, Roman Pohrt, Iakov A Lyashenko, and Valentin L Popov. Boundary element method for nonadhesive and adhesive contacts of a coated elastic half-space. 234(1): 73–83. ISSN 1350-6501. doi: 10.1177/1350650119854250.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Data-driven finite-thickness cohesive elements for frictional interfaces

S. Z. Wattel [†*], J. Garcia-Suarez[†] and J.-F. Molinari[†]

[†] Institute of Civil Engineering, Institute of Materials
École Polytechnique Fédérale de Lausanne (EPFL)
Lausanne, Switzerland

[*] Email: sacha.wattel@epfl.ch

Abstract: Model-free data-driven computational mechanics (DDCM) [**Kirchdoerfer & Ortiz, 2016**] is a new paradigm for simulations in solid mechanics. As in the classical method, the boundary value problem is formulated with physics-based PDEs such as the balance of momentum and compatibility equations, which together define the admissibility conditions. However, DDCM does not use phenomenological constitutive laws to close the problem. Instead it uses directly data on material response, originating from either experiments or micro-physical simulations, in order to reduce constitutive modeling bias. The problem is solved in phase space where the admissibility conditions define a manifold and the material behavior is represented by a set of material points. DDCM aims to find the admissible state that best matches the material points. The DDCM framework has been formulated and used to solve problems in statics and dynamics, for multi-scale modeling, and has been coupled to classical solvers such as the finite element method to run simulations more efficiently. In this work, DDCM is applied to a frictional interface. Data-driven finite-thickness cohesive elements are sandwiched between two linear elastic bodies solved with FEM. The material response database is populated from micro-physical discrete simulations of two contacting rough surfaces sliding against each other. Through interactions between the interface, the bulk and the boundary conditions, complex behaviors such as dynamically propagating slip fronts arise.

Keywords: Data-Driven Computational Mechanics, Tribology, Frictional Interface

[**Kirchdoerfer & Ortiz, 2016**] 'Data-driven computational mechanics', CMAME, 2016

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical generation of random rough surfaces using Generative Adversarial Networks

T. R. Silva Sabino[*†1], **A. M. Couto Carneiro**[*†2], **R. Pinto Carvalho**[†3], **F. M. Andrade Pires**[*†4]

[*] Department of Mechanical Engineering (DEMec)
Faculty of Engineering of the University of Porto
Porto, Portugal

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

[1]e-mail: sabino@fe.up.pt; [2]e-mail: amcc@fe.up.pt; [3]e-mail: rpcarvalho@inegi.up.pt; [4]e-mail: fpires@fe.up.pt

Abstract:

In the current engineering landscape, roughness is not considered a secondary effect anymore. It occupies an important place in recent technological advances, as it is typically related to the efficiency and durability of the equipment. It has been extensively demonstrated that roughness plays a paramount role in friction, electrical and thermal contact resistance, wear, adhesion, among many others [1]. The acknowledgement of roughness as an important engineering phenomenon and the many research advances on the topic has only been possible due to the efforts put into the characterization and description of rough surfaces. As a result, the artificial generation of rough surfaces has conquered an important place and has become an attractive research topic, over the recent past [2].

The introduction of data-driven models to analyse rough topographies has been gaining traction in the last decade. These can outperform the traditional techniques on the overall computational cost and are able to easily deal with real surface measurements. In this research, Generative Adversarial Networks (GANs [3]) are applied to generate random rough surfaces using the Power Spectral Density (PSD) for the parameterisation. To this end, the training process is improved to guide the generator model towards the correct PSD beyond the standard similarity metrics used in these types of machine learning techniques. The methodology is validated by assessing the mechanical response of the newly generated surfaces through numerical simulations for rough contact. This study reveals interesting insights and potential applications of GANs for the generation of complex random topographies that can be found in real-life applications.

Keywords: Rough surfaces, Roughness generation, Generative Adversarial Networks, Convolutional Neural Networks, Real contact area

References:

[1] R. Aghababaei, E. E. Brodsky, J.-F. Molinari, and S. Chandrasekar, ‘How roughness emerges on natural and engineered surfaces’, *MRS Bull.*, Jan. 2023, doi: 10.1557/s43577-022-00469-1.
[2] P. Pawlus, R. Reizer, and M. Wieczorowski, ‘A review of methods of random surface topography modeling’, *Tribol. Int.*, vol. 152, p. 106530, Dec. 2020, doi: 10.1016/j.triboint.2020.106530.
[3] I. J. Goodfellow *et al.*, ‘Generative Adversarial Networks’. arXiv, Jun. 10, 2014. doi: 10.48550/arXiv.1406.2661.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Rough Contact of Inelastic Materials: Viscous Effects

Vladislav A. Yastrebov

Mines Paris, PSL university, Centre des matériaux, CNRS UMR 7633, Evry, France
e-mail: vladislav.yastrebov@minesparis.psl.eu

Abstract: Mains trends in mechanical contact of rough surfaces of inelastic materials are relatively well understood. However, in this work, we make an attempt to construct a quantitative link of physically relevant contact properties with roughness features (height distribution, fractal dimension) and loading parameters (duration, cycling, normal or tangential loading). Notably, we study viscous effects in elastomers and metals by means of advanced finite element simulations. Relevant phenomena such as friction, wear, permeability to fluids, thermal and electric resistance are also discussed in the context of obtained results.

Keywords: Contact, roughness, visco-plasticity, visco-elasticity, FEM, time dependence, friction

1 Introduction

Most of engineering systems are designed to operate in elastic regimes at least at the structural scale and within the assumption of homogeneity of materials, the same holds for the mechanical contact between the components of such systems. However, it is not always the case at the microstructural scales at which the surface roughness has to be taken into account. At these scales, the material can experience much higher loads than those nominally computed for homogeneous and smooth surfaces. Such loads often induce stress-strain states far beyond the elastic regime. Moreover, for many materials and their combinations the hold time and the sliding velocity can affect considerably tribological properties of the interface. The objective of this study is to better understand how such an inelastic material behavior influences some fundamental quantities in physics of rough surfaces such as the evolution and morphology of the true contact area and the gap. The special attention will be paid to viscous effects related to hold time and sliding velocity.

1.1 Methods

To study the strongly nonlinear emerging problem we use the finite element suite Z-set [1] capable to handle all material non-linearities with the state of the art surface-to-surface contact discretization and advanced monolithic solvers and particular algorithms for treatment of such complex coupled non-linear problems. The following materials will be considered: (1) isotropic von Mises elasto- plastic material with both kinematic and isotropic hardening (most of metal and alloys), see Fig. 1, (2) visco-elastic material taking into account Payne effect, (3) visco-plastic material with zero threshold non-linear flow, equivalent to Glen's rheology of ice.

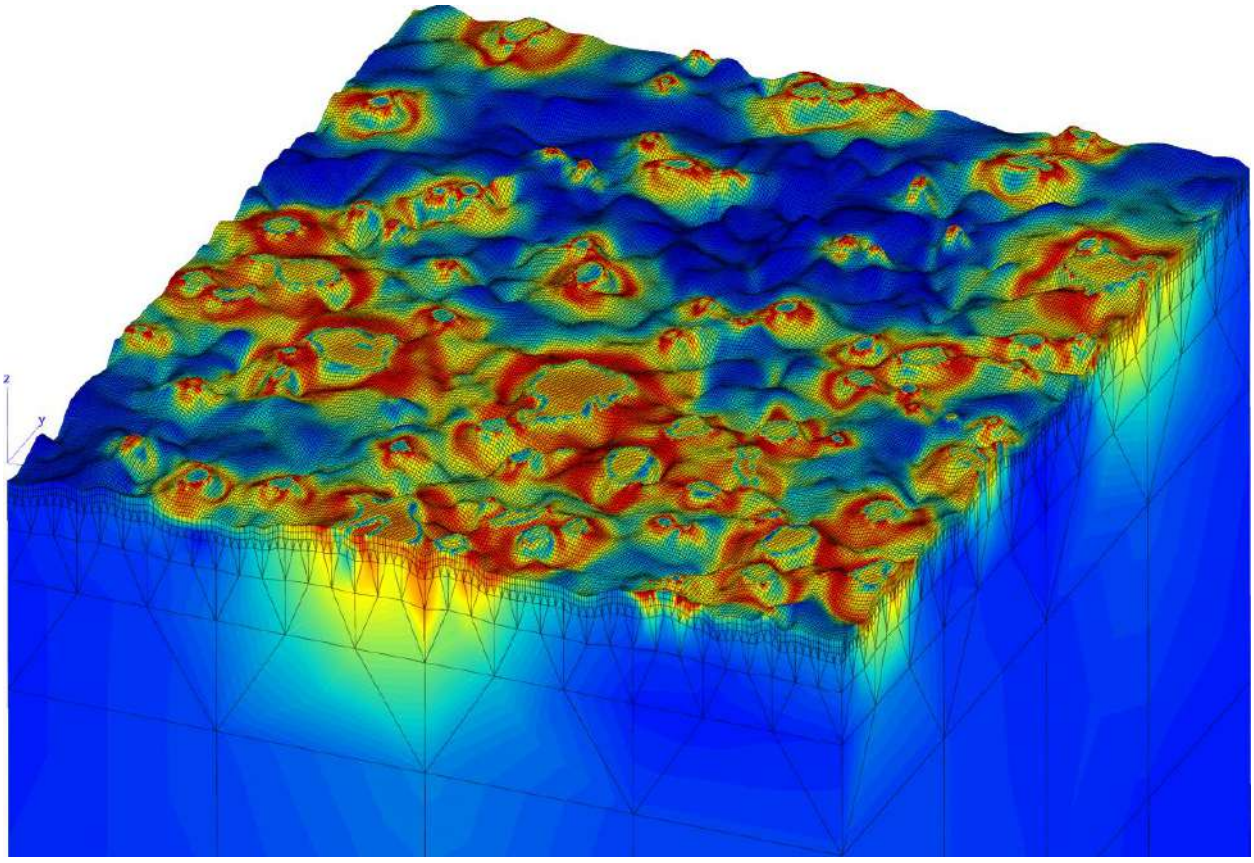


Figure 1: von Mises stress distribution after unloading of a rough metallic surface after contact with a rigid flat [2].

2 Results & Discussion

This study is focused on the effect of hold time and sliding velocity in contact of rough surfaces made of viscoelastic and viscoplastic material. In particular, we investigate the growth of the friction during the hold under constant load and reveal the physics of microscopical processes leading to this growth. Regardless a huge difference in physics of viscoelasticity and rate-dependent plasticity, the contact-related behavior on small scales is shown to be very similar. However, when rough solids slide one past to another, the physics of these two types of materials is very different. Interesting qualitative and quantitative results will be demonstrated which are important for fundamental understanding of microscopic processes.

References

[1] Finite Element Suite Z-set, www.zset-software.com (2022).

[2] Yastrebov, V.A. et al., "Rough surface contact analysis by means of the Finite Element Method and of a new reduced model". Comptes Rendus Mecanique, 339:473-490 (2011).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Design of truss and frame structures using alternative performance indicators

Nicolai Grünvogel*, David Forster*, Malte von Scheven*, Manfred Bischoff*

* University of Stuttgart
Institute for Structural Mechanics
Stuttgart, Germany
e-mail: {gruenvogel; forster; mvs; bischoff}@ibb.uni-stuttgart.de

Abstract: For the design of efficient, sustainable, and safe structures it is often helpful to use alternative performance indicators compared to displacements and stresses for structural evaluation and decision-making. The redundancy matrix provides a detailed and valuable insight into the structural behaviour of statically indeterminate structures. It can be used in the early design phase of truss and frame structures to achieve robustness and to estimate the imperfection sensitivity at an early design stage and independent of the load. The deformation modes and redundancy distribution for trusses and beams will be discussed shortly. Interpretation and application of the redundancy matrix as a basis for alternative structural performance indicators are the main highlights. These can assist in choosing the optimum design in terms of for instance reliability, robustness and sensitivity to imperfections.

Keywords: redundancy matrices, alternative structural performance indicators, numerical design

1 Introduction

One of the overarching goals of the Cluster of Excellence Integrative Computational Design and Construction for Architecture is to improve cooperation between architecture, engineering, and practical manufacturing as so-called "Co-Design"[1]. This should enable a better feedback-loop for the entire design process. To this end, civil engineering is trying to find and apply alternative evaluation methods in order to improve the design process to conserve resources and reduce the material costs. Deformations, strains, and stresses are well known as performance indicators of a structural system, which are load-dependent. For an early assessment of different design variants, alternative indicators can be used, based on the redundancy matrix introduced by Bahndorf [2]. Among others, it describes the distribution of the static indeterminacy within a given structure independent of the applied load, aiding in the identification of potentially critical structural parts.

2 Redundancy in truss and beam structures

In von Scheven et al. [3] a detailed study on the redundancy distribution for trusses and beams is given. The redundancy matrix $\mathbf{R}$ maps the initial elongations $\Delta\mathbf{l}_0$ to the negative elastic elongations $\Delta\mathbf{l}_{\mathrm{el}}$.

$$-\Delta\mathbf{l}_{\mathrm{el}} = \mathbf{R}\Delta\mathbf{l}_0 \quad \mathbf{R} = \Delta\mathbf{l} - \Delta\mathbf{l}_0 = \mathbf{I} - \mathbf{A}\mathbf{K}^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{C}, \tag{1}$$

where $\mathbf{A}$ is the compatibility matrix, $\mathbf{C}$ is the member stiffness matrix, and $\mathbf{I}$ is the identity matrix. The diagonal entries describe the distribution of static indeterminacy in the structure. For truss elements, the values are between 0 and 1, where $r_{ii} = 0$ describes a statically determinate element with no redundancy. The trace of the redundancy matrix $\mathrm{tr}(\mathbf{R})$ is equal to the degree of static indeterminancy of the system. The extension to beam elements is

straightforward, but instead of only one deformation mode, as in the truss element, elongation, there are three deformation modes due to the additional shear and bending parts. The image of the redundancy matrix $\mathrm{im}(\mathbf{R})$ and the kernel $\ker(\mathbf{R})$ both span a space with special properties, like for instance purely incompatible elongation modes in a structure. For more details see von Scheven et al. [3].

3 Interpretation and Application

The entries of $\mathbf{R}$ can also be interpreted as a measure for the sensitivity to imperfections, since they quantify the constraint that the surrounding structure imposes on an individual element. In order to have a robust and reliable structure with no statically determinate parts, the redundancy of an element should never be zero. On the other hand, small values of redundancy will lead to the small forces in the structure brought on by manufacturing-related imperfections, and might be therefore advantageous during assembly processes in some specific areas. Some examples will be discussed in this domain utilizing the characteristics of the redundancy matrix to obtain an improved design.

4 Conclusion

Alternative performance indicators, based on the redundancy matrix can be used in the design of truss and frame structures to improve overall performance and identify any potentially critical substructures in statically indeterminate structures. It also gives valuable insights into the load-carrying behaviour both on a global structural and on a local element level. There is work in progress with regard to the Co-Design of fiber-reinforced structures, with the aim to develop and optimize large-scale structures in terms of sustainability, assemblability, and increasing efficiency in design and construction.

5 Acknowledgements

This research was supported by the Deutsche Forschungsgemeinschaft (DFG; German Research Foundation) under Germany's Excellence Strategy – EXC 2120/1 – 390831618.

References

[1] Gil Pérez, M., Zechmeister, C., Kannenberg, F., Mindermann, P., Balangé, L., Guo, Y., Hügle, S., Gienger, A., Forster, D., Bischoff, M., Tarín, C., Middendorf, P., Schwieger, V., Gresser, G.T., Menges, A., Knippers, J., 2022. Computational co-design framework for coreless wound fibre–polymer composite structures. Journal of Computational Design and Engineering 9(2), 310-329.

[2] Bahndorf, J., 1991. Zur Systematisierung der Seilnetzberechnung und zur Optimierung von Seilnetzen, Deutsche Geodätische Kommission bei der Bayerischen Akademie der Wissenschaften Reihe C, Dissertationen. Verlag der Bayerischen Akademie der Wissenschaften, München.

[3] von Scheven, M., Ramm, E., Bischoff, M., 2021. Quantification of the redundancy distribution in truss and beam structures. International Journal of Solids and Structures 213, 41–49.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

The story behind a blind prediction of a 3-storey infilled reinforced concrete building

André Furtado[*], Hugo Rodrigues[†1], António Arêde[†2] and Humberto Varum[†3]

[*] CERIS – Instituto Superior Técnico de Lisboa
Universidade de Lisboa
Lisboa, Portugal
e-mail: andre.furtado@tecnico.ulisboa.pt

[†1] RISCO – Universidade de A
Aveiro, Portugal
e-mail: hrodrigues@ua.pt

[†2] CONSTRUCT – Faculdade de Engenharia da Universidade do Porto
Porto, Portugal
e-mail: aarede@fe.up.pt

[†3] CONSTRUCT – Faculdade de Engenharia da Universidade do Porto
Porto, Portugal
e-mail: hvarum@fe.up.pt

Abstract: Over the last few years the seismic behaviour of infilled reinforced concrete (RC) structures has been the focus of numerous experimental and numerical studies. A big effort is being made by the scientific community with the aim of increasing the knowledge regarding the seismic response of these types of structures and improving the numerical modelling accuracy to predict their expected behaviour. In 2015, a blind prediction contest was organized by the Faculty of Civil Engineering Osijek with the main goal of inviting the technical and scientific community to predict the nonlinear seismic behaviour of a 1:2.5 scaled 3D building structure. The three-storey infilled RC structure was subjected to ten incremental earthquake sequences on a shake table test. The blind numerical analyses were performed knowing only the specimen geometry, reinforcement detailing, material characteristics and the actual ground motions recorded during the testing. In this context and, in view of the author's participation success, the present paper mainly aims at presenting the key aspects of the adopted numerical methodology (and related difficulties) which proved to yield good results, while also providing some insight regarding key problems in numerical simulations of infilled RC structures seismic behaviour.

Keywords: Blind Prediction, infilled RC structures, Seismic behaviour, Numerical modelling

1. INTRODUCTION

In the context of seismic scientific testing, works developed in the last years and in particular resorting to shaking tables, which usually happens with the objective of providing additional information not available from simpler experimental tests. In 2015, the FRAmed–Masonry Composites for Modeling and Standardization (FRAMA) Blind Prediction Contest 2014 [1] pretended to evaluate different modelling strategies proposed by different international teams/experts that were challenged to predict the experimental response of a scaled three-storey infilled RC structure that will be subjected to ten increased and scaled ground motions where the authors team became in the first position. This research work aims at describing the modelling strategy adopted by the author in terms of the RC structure and infills masonry walls modelling.

2. MAIN RESULTS

The experimental program associated with the FRAMA Blind Prediction Contest [1] initiative was performed in DYNLAB at IZIIS shaking table with the support of University of Osijek (Croatia) and is briefly described in this chapter. It basically involved of a 1:2.5 scaled infilled RC structure (Figure 1) under uniaxial ground motions with increasing intensity. The shake-table test specimen was a 1:2.5 scale model that contains two parallel connected planar frames, with two bays and three storeys, making the structure of the gross dimensions of 4.6 m in length, 2.8 m in width and 3.9 m in height. The RC structured is filled with masonry walls with openings in certain bays. The structure has been designed for medium ductility levels according to the EC8 provisions

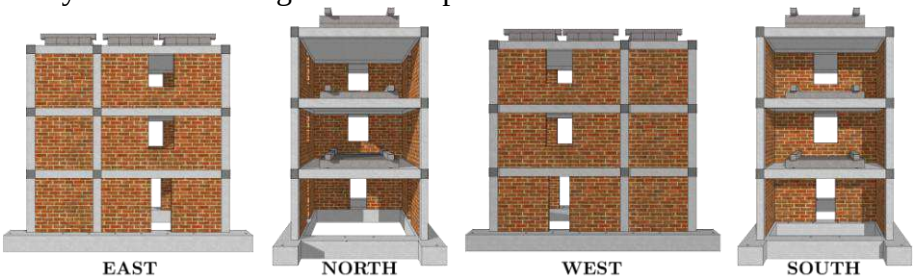
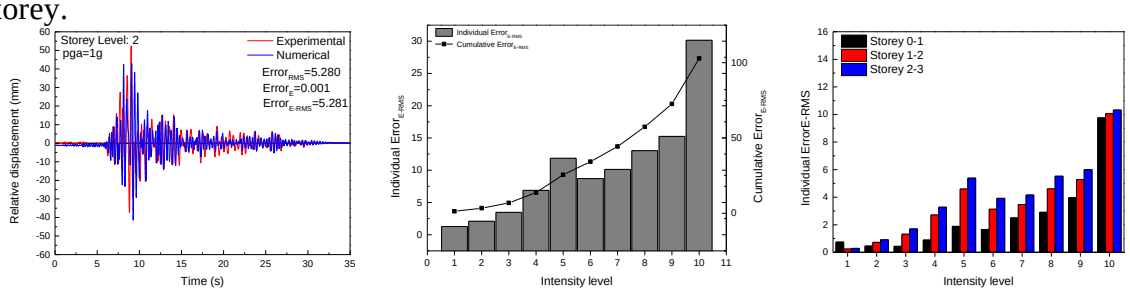


Figure 1 – 3 storey masonry-infilled RC frame and reinforcement details Lateral views.

Figure 2 shows the comparison between the experimental and numerical relative displacements. It can be observed in Figure 2b that the error obtained on 5 different levels was lower than 10 and only for pga=1.2g the error was higher than 30. The error is progressively increasing with the increasing pga demand, however for pga=0.4g the error is slightly above of those observed before which reach an $Error_{E\text{-}RMS}$=11.86. It can be observed that the error obtained in the prediction of the 3rd storey displacement is around 2-2.5 times higher than the obtained for the 1st storey and 1.25-1.5 times the ones achieved for the 2nd storey.



a) b) c)

Figure 2 – Main results: a) relative displacement; b) invidual error; and c) individual erro per intensity level.

Acknowledgements

The author is grateful for the Foundation for Science and Technology's support through funding UIDB/04625/2020 from the research unit CERIS.

References

[1] V. Sigmund *et al.*, "FRAmed–MAsonry Composites for Modeling and Standardization, FRAMA, International Benchmark within Research Project, Faculty of Civil Engineering Osijek, Josip Juraj Strossmayer University of Osijek, Croatia,," 2014.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modal strain-based SHM of steel railway bridges

Anastasopoulos Dimitrios*, Reynders Edwin P.B. †

* Department of Civil Engineering
Faculty of Engineering Science, KU Leuven
Leuven, Belgium
e-mail: dimitrios.anastasopoulos@kuleuven.be

† Department of Civil Engineering
Faculty of Engineering Science, KU Leuven
Leuven, Belgium
e-mail: edwin.reynders@kuleuven.be

Abstract: Natural frequencies are the most widely used modal characteristics in vibration-based monitoring. However, they can be highly influenced by temperature and this influence can completely mask the effect of damage. Displacement mode shapes are less sensitive to temperature, but obtaining them in a dense grid, a requirement for damage localization, is cumbersome due to the large number of sensors needed. Strain mode shapes on the other hand can be nearly insensitive to temperature, while obtaining them in a dense grid is possible when fiber-Bragg gratings (FBG) are used. This work presents an overview of the continuous modal strain-based monitoring of three steel railway bridges of different structural typologies. All bridges were instrumented with FBGs and their strain mode shapes were automatically obtained on an hourly basis from ambient and operational dynamic strains. The influence of temperature on the strain mode shapes is investigated and their low sensitivity to temperature is confirmed for all bridges. The damage detection and localization capabilities of the strain mode shapes are also demonstrated numerically and experimentally.

Keywords: modal strains, vibration-based monitoring, environmental influence, damage localization

1 Introduction

Strain mode shapes [1] are an advantageous alternative to displacement mode shapes for vibration-based monitoring (VBM) [2]. Strain mode shapes consist of modal strains, similarly to the conventional displacement mode shapes, which consist of modal displacements. Modal strains are obtained from dynamic strain measurements. Dense strain sensor grids can be easily achieved when fiber-Bragg gratings (FBG) are employed, due to their multiplexing possibility. Modal strains are generally much more sensitive to local damage than modal displacements and less sensitive to temperature than natural frequencies [2, 1]. Laboratory experiments on concrete beams have illustrated these advantages [1].

The assessment of the strain mode shapes' performance in situ has remained an open problem until recently. This work presents the results, conclusions and lessons learned from the continuous dynamic strain monitoring with FBGs of three steel railway bridges of different structural typology. The natural frequencies and the strain mode shapes of these bridges were automatically identified on an hourly basis through the method that was developed and described in [3], in order to evaluate their condition. The influence of temperature on the monitored quantities is assessed, as well as the influence of real-life and simulated damage.

2 Modal strain-based monitoring of railway bridges

A steel Vierendeel arch bridge, a steel tied-arch bridge and a steel riveted beam bridge have been monitored in the course of the past four years. The bridges are shown in Figure 1.

Figure 1: Left: The Vierendeel arch bridge (Mechelen, Belgium). Center: The KW51 tied-arch bridge (Leuven, Belgium). Right: The Nieuwebrugstraat riveted beam bridge (Ronse, Belgium).

The same observations were made for all bridges, regardless of their type. First, the strain mode shapes of all identified modes were found to be insensitive to temperature changes higher than 0°C. Exception are the strain mode shapes of the higher order modes of the KW51 bridge, which were found to be sensitive to frost, due to the freezing of the ballast layer. However, this influence was significantly smaller than the influence that was observed on natural frequencies due to frost and most importantly, to the influence of small-scale, simulated damage on the strain mode shapes. Second, the natural frequencies of all modes were found to be influenced by temperature. The change in natural frequency due to the change in temperature was higher than the change imposed by small-scale damage in both simulated and real-life damage cases. This underlines the necessity of damage normalization, before using the natural frequencies for monitoring purposes. Third, contrary to natural frequencies, strain modes shapes were highly sensitive to small-scale damage that occurred in the vicinity of the monitored locations, an outcome that combined with their temperature insensitivity renders them ideal for direct damage assessment.

3 Conclusions

The observations from these three case-studies demonstrate the high potential of strain mode shapes for damage detection and localization and consequently, for the practical VBM.

References

[1] Anastasopoulos D, De Roeck G, Reynders E. Influence of damage versus temperature on modal strains and neutral axis positions of beam-like structures. Mech Syst Signal Proc 2019;134:106311.

[2] Fan W, Qiao P. Vibration-based damage identification methods: a review and comparative study. Struct Health Monit 2010;10(1):83–111.

[3] Anastasopoulos D, De Roeck G, Reynders E. One-year operational modal analysis of a steel bridge from high-resolution macrostrain monitoring: influence of temperature vs. retrofitting. Mech Syst Signal Proc 2021;161:107951.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Model for steel fibre reinforced concrete panels subjected to in-plane shear stresses

Rui Valente[*], Mário Pimentel[†]

[*] Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: rui.v@fe.up.pt

[†] Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: mjsp@fe.up.pt

Abstract: This paper presents a mechanical model for analyzing the shear behavior of cracked concrete panels containing both steel fibers and rebars (R-FRC). The model is based on the Cracked Membrane Model [1, 2] with fixed and interlocked cracks. The model is validated with experimental results.

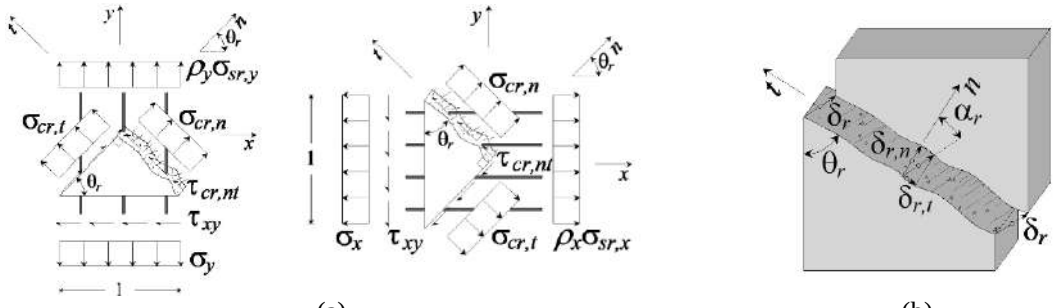
Keywords: Constitutive model, fibre-reinforced concrete, panels, plane stress, shear strength

1. Introduction

Steel fibres could be used as replacement for conventional shear reinforcement in concrete elements. However, the interaction between rebars and fibres is not fully understood as well as their relative contributions for shear strength. Therefore, the goal of this work is the development of a theoretical model capable of describing the complex mechanics and capturing the full behaviour of cracked R-FRC panel elements under pure shear stresses.

2. Methods

The model developed in [2] is adapted to account for the fibres contribution at the cracks and is based on equilibrium and compatibility of deformations.



(a) (b)

Figure 1. (a) Equilibrium expressed in terms of stresses at the crack and (b) crack kinematics and notation

The equilibrium is established at the crack level (Figure 1 (a)). The crack stresses are found by means of constitutive laws as function of the panel total strains. The rebar stresses at the cracks (σ_{sr}) are related to the total average strains by means of the TCM equations [3]. The stresses normal to the crack ($\sigma_{cr,n}$) are obtained by summing the crack dilatancy stresses arising from the crack shear transfer mechanisms (σ_{dil}) and the normal component of fibres

bridging stresses (σ_{cfn}). The crack shear stress is given by the sum of the shear stresses arising from the aggregate interlock (τ_{agg}), and tangential component of fibre bridging stresses (σ_{cft}). The fibre bridging stresses at the cracks are determined using fibre engagement models [4] as a function of the crack displacement (δ_r) (Figure 1 (b)). The stresses due to interlock effects are rmined using the Contact density model [5] as a fcuntions of the crack openin ($\delta_{r,n}$) and slip ($\delta_{r,t}$).

3. Validation

The experimental results [6] on R-FRC panels tested under in-plane pure-shear monotonic loading conditions are used to validate the proposed theoretical model (Figure 2). Different fibre content (V_f) and fibre geometries, described by their length (l_f) and diameter (d_f), are used. The increasing shear strength with increasing fibre content (V_f) observed in experimental results is captured by the model. However, the increase is not as significant from C1F1V2 to C1F1V3 in the exeperimental results.

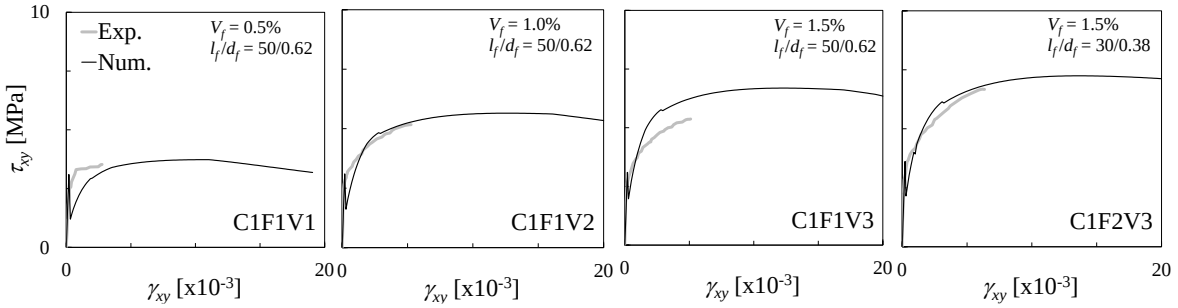


Figure 2. Comparison of calculated and experimental shear stress-strain curves of R-FRC panels tested under in plane shear

3. Conclusions

This paper presents a fixed crack model for the analysis of R-FRC cracked membrane elements subjected to in-plane shear. The model results are satisfactorily compared with available test experimental data. The model will be simplified to code-like formulation to serve as basis fot the design of R-FRC elements.

References

[1] Kaufmann, W. and P. Marti, *Structural concrete: cracked membrane model.* Journal of materials in civil engineering, 1998. **124**(12): p. 1467-1475.

[2] Pimentel, M., E. Brüwhiler, and J. Figueiras, *Extended cracked membrane model for the analysis of RC panels.* Engineering Structures, 2010. **32**(8): p. 1964-1975.

[3] Marti, P., et al., *Tension chord model for structural concrete.* Structural Engineering International, 1998. **8**(4): p. 287-298.

[4] Pfyl, T., *Tragverhalten von stahlfaserbeton*, in *Institut für Baustatik und Konstruktion*. 2003, Eidgenössische Technische Hochschule Zürich: Zürich.

[5] Li, B., K. Maekawa, and H. Okamura, *Contact Density Model for Stress Transfer across Cracks in Concrete.* Journal of the Faculty of Engineering of Tokyo, 1989. **XL**(1): p. 9-52.

[6] Susetyo, J., *Fibre reinforcement for shrinkage crack control in prestressed, precast segmental bridges*, in *Graduate Department of Civil Engineering*. 2009, University of Toronto: Toronto.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Investigating the fatigue behaviour of Puddle Iron Retrofitting solutions through Experimental and Numerical approaches

João Arrojado[1], Anis Mohabedine[2], José A.F.O. Correia[3], Diogo Ribeiro[4], Anna Racokzy[5]

[1] Ph.D. Student, CONSTRUCT, Faculty of Engineering, University of Porto, Portugal
e-mail: up201606508@fe.up.pt

[2] Researcher, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands
e-mail: a.i.mohabeddine@tudelft.nl

[3] Researcher, CONSTRUCT, Faculty of Engineering, University of Porto, Portugal
e-mail: jacorreia@fe.up.pt

[4] Assistant Professor, CONSTRUCT, School of Engineering, Polytechnic of Porto, Portugal
e-mail: drr@isep.ipp.pt

[5] Assistant Professor, Institute of Roads and Bridges, Department of Civil Engineering, Warsaw University of Technology, Poland
e-mail: anna.racokzy@pw.edu.pl

Introduction

All over Europe, railway transport underwent substantial development at the beginning of the 20th century with the construction of many riveted metallic bridges. Different design and execution techniques have developed as the materials used to build them and it can contribute to a better understanding of these structures' behaviour. These bridges will have their operational life extended over time, making it necessary to carry out studies to evaluate the remaining lifespan, in order to assess economic concerns. Furthermore, the traffic volume and axle loads have been increasing, then residual life studies are so relevant. In the particular case of metallic and composite bridges, several authors describe fatigue as being the principal cause of several damages [1], [2]. Traditional fatigue design rules aren't suitable for old metallic bridges, don't carry all the types of riveted and bolted joints, and, moreover, don't consider multiaxial stress states for both crack initiation and propagation phases. Also, fatigue assessment methods from codes and regulations based on global S-N curves conduct very conservative predictions [3]. In Portugal, experimental studies were carried out on metallic old bridges' materials, collecting data about mechanical properties, chemical composition, and microstructures [4]. Alternative fatigue approaches were done by authors: S-N curves were proposed based on probabilistic models and monotonic and fatigue experimental data calibrated with numerical Finite Element models [5]. In order to increase fatigue life, CFRP (Carbon Fiber Reinforced Polymers) has been studied as a retrofitting solution, showing a high strength-to-weight ratio, good behaviour to corrosion, and very good performance under fatigue loading, retarding crack propagation and extending fatigue life [6], [7].

This paper presents an experimental campaign on puddle iron from Luiz I bridge under static and fatigue conditions, and numerical modelling approaches to predict fatigue life using Finite Element Analysis (FEA) software ABAQUS®.

Keywords: Metallic bridges, monotonic behaviour, fatigue, retrofitting, CFRP.

Acknowledgements

This work was financially supported by: Project PTDC/ECI-EST/30103/2017 - POCI-01-0145-FEDER-030103 - funded by FEDER funds through COMPETE2020 - Programa Operacional Competitividade e Internacionalização (POCI) and by national funds (PIDDAC) through FCT/MCTES. This research was also supported by CONSTRUCT - Instituto de I&D em Estruturas e Construções that is funded by base funding - UIDB/04708/2020 and programmatic funding - UIDP/04708/2020 provided by national funds through the FCT/MCTES (PIDDAC). João Arrojado would like to thank the Ph.D. research grant (2022.13575.BD) awarded by national funds (PIDDAC) through the Portuguese Science Foundation (FCT/MCTES). José A.F.O. Correia would like to thank the individual project grant (2020.03856.CEECIND) awarded by national funds (PIDDAC) through the Portuguese Science Foundation (FCT/MCTES).

References

[1] J. W. Fisher and S. Roy, "Fatigue of steel bridge infrastructure," *Struct. Infrastruct. Eng.*, vol. 7, no. 7–8, pp. 457–475, 2011, doi: 10.1080/15732479.2010.493304.

[2] A. M. P. d. Jesus, A. L. L. d. Silva, and J. A. F. O. Correia, "Fatigue of riveted and bolted joints made of puddle iron - A numerical approach," *J. Constr. Steel Res.*, vol. 102, pp. 164–177, 2014, doi: 10.1016/j.jcsr.2014.06.012.

[3] S. P. Zhu, Z. Y. Yu, J. Correia, A. De Jesus, and F. Berto, "Evaluation and comparison of critical plane criteria for multiaxial fatigue analysis of ductile and brittle materials," *Int. J. Fatigue*, vol. 112, no. February, pp. 279–288, 2018, doi: 10.1016/j.ijfatigue.2018.03.028.

[4] A. M. P. d. Jesus, A. L. L. d. Silva, M. V. Figueiredo, J. A. F. O. Correia, A. S. Ribeiro, and A. A. Fernandes, "Strain-life and crack propagation fatigue data from several Portuguese old metallic riveted bridges," *Eng. Fail. Anal.*, vol. 18, no. 1, pp. 148–163, 2011, doi: 10.1016/j.engfailanal.2010.08.016.

[5] J. Correia *et al.*, "Fatigue crack growth modelling of Fão Bridge puddle iron under variable amplitude loading," *Int. J. Fatigue*, vol. 136, no. January, p. 105588, 2020, doi: 10.1016/j.ijfatigue.2020.105588.

[6] A. Mohabeddine, J. A. F. O. Correia, P. A. Montenegro, and J. M. Castro, "Fatigue crack growth modelling for cracked small-scale structural details repaired with CFRP," *Thin-Walled Struct.*, vol. 161, p. 107525, Apr. 2021, doi: 10.1016/j.tws.2021.107525.

[7] X. L. Zhao and L. Zhang, "State-of-the-art review on FRP strengthened steel structures," *Eng. Struct.*, vol. 29, no. 8, pp. 1808–1823, Aug. 2007, doi: 10.1016/j.engstruct.2006.10.006.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Probabilistic Fatigue Analysis of Metallic Bridge Riveted Connection under Linear and Non-Linear Accumulation Rules

Mourão, A.[1]; Silva, João Nuno[2]; Horas, Cláudio[3]; Correia, J.A.F.O.[4] ; Bittencourt, Túlio[5] ; Calçada, Rui[6]

[1] Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: amourao@fe.up.pt

[2] Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: up201705111@edu.fe.up.pt

[3] Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: claudiohoras@fe.up.pt

[4] Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: jacorreia@fe.up.pt

[5] Polytechnical School, Universidade de São Paulo
São Paulo, Brazil
e-mail: tbitten@usp.br

[6] Department of Civil Engineering (DEC)
Faculdade de Engenharia, Universidade do Porto
Porto, Portugal
e-mail: ruiabc@fe.up.pt

Abstract: The importance of the fatigue phenomenon in engineering (e.g., bridges) is widely recognized and has been the cause of major collapses in recent decades, either due to a mindset of neglect resulting in poor maintenance strategies, increasing traffic demands both in frequency and magnitude, exposure to aggressive environmental agents, amongst others.

From an European perspective roughly 200 000 metallic bridges have been identified to be at risk of collapse, a number which pales in comparison with the 3 fold in the United States under the same operational conditions. Either due to cultural or socioeconomical constraints, a wide range of these critical infrastructure see their operational life extended behond what was originally planned, leading to fatigue accumulation. Hence, accurate and reliable fatige assessment and consequent service life estimations are highly relevant, even though a complex task to achieve in a real-word scenario given the high-dimensionality of the problem.

Several models can be implemented with aims to determine fatigue life; however, the reliability of such methodologies depends not only on the concentrations of stress/strains, multiaxiality, size effects, but also the model's ability to grasp the behaviour of the joints under multi-level loading scenarios.

As such, this work focuses on the compound effect that both chosen probabilistic analysis, used to obtain design fatigue strength curves for the Várzeas bridge riveted connection, as well as the fatigue accumulation rules play in the final fatigue assessment of the structure. For this, several probabilistic methodologies were employed, standardized (ISO & ASTM), probabilistic approach based on the 2-parameter Weibull probability density function, all of whom fitted using classic and total least squares methods. Additionally, the Castillo and Fernández-Canteli based on the 3-parameter Weibull distribution as well as the Markov-Chain Monte Carlo were used. Finally, both linear and non-linear damage accumulation rules, namely the Sequential Law and Huffman models were taken into consideration, the latter group to account for loading sequence effects.

Keywords: Bridge, Riveted Connections, Probabilistic Modelling, Fatigue Accumulation

Acknowledgements

This research was supported by: project grant (PTDC/ECI-EST/30103/2017) FiberBridge - Fatigue strengthening and assessment of railway metallic bridges using fiber-reinforced polymers by FEDER funds through COMPETE2020 (POCI) and by national funds (PIDDAC) through the Portuguese Science Foundation (FCT/MCTES); and, base funding - UIDB/04708/2020 and programmatic funding - UIDP/04708/2020 of the CONSTRUCT - Instituto de I&D em Estruturas e Construções - funded by national funds through the FCT/MCTES (PIDDAC). António Mourão would like to thank the Ph.D. research grant (PD/BD/150306/2019) awarded by national funds (PIDDAC) through the Portuguese Science Foundation (FCT/MCTES). The author João Silva gratefully acknowledges the financial support by MIT- EXPL/SOE/0054/2021 - Hyperloop-Verne - Exploratory Analysis of Biomimetic-inspired Oceanic Hyperloop Transport Infrastructures. José Correia would like to thank the individual project grant (2020.03856.CEECIND) awarded by national funds (PIDDAC) through the Portuguese Science Foundation (FCT/MCTES).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

IGA-based topology optimization of compliant mechanisms

Villalba D. [*] [†], Gonçalves M.[*] , Dias de Oliveira J.[*], Andrade-Campos A.[*] and Valente R.[*]

[*] Departamento de Engenharia Mecanica (TEMA)
Campus de Santiago, Universidade de Aveiro
Aveiro, Portugal
e-mail: diego.villalba/mafalda.goncalves/jalex/gilac/robertt@.ua.pt

[†] Escuela Técnica Superior de Ingeniería de Caminos, Canales y Puertos (ETSICCP)
Campus de Elviña, Universidade da Coruña
A Coruña, España
e-mail: diego.villalba.rama@udc.es

Abstract: In this research, an isogeometric formulation of the material distribution for the topology optimization of compliant mechanisms is proposed. The aim of this formulation is to provide solutions with high spatial definition by using a lower number of design variables in comparison with the classical formulations used to define the material layout. The structural analysis considered is linear and it is performed by means of the Isogeometric Analysis (IGA). The distribution of the material in the domain is modeled with quadratic B-splines. The proposed formulation of the topology optimization problem of compliant mechanisms is tested by means of a benchmark problem. This problem is also solved with a Finite Element (FEM) formulation to compare with the IGA-based solutions. In the FEM-based formulation, the relative density is uniform at each element of the mesh. The attained results show that the IGA-based formulation provides solutions with high spatial definition in comparison with the FEM-based formulation. A better representation of the topology contour and a mitigation of the mesh dependence phenomena is attained with the use of IGA. Despite of this improvements both solutions are topologically equivalent.

Keywords: Topology Optimization, Compliant Mechanisms, FEM, IGA

1 Introduction

The use of the topology optimization in the design of compliant mechanisms has been developed by [1, 2]. An important number of contributions in the topology optimization field by using the isogeometric formulations have been made [3, 4]. However, the solution of the topology optimization problem of compliant mechanisms by using the isogeometric formulations has not been widely studied. Consequently, this is the main objective of this research since solutions with high spatial definition are intended.

2 Problem formulation

The conventional topology optimization problem of compliant mechanisms can be stated as:

$$\max \; T(\boldsymbol{\rho}) = u_{\text{out}}(\boldsymbol{\rho}) \qquad \text{s.t.} \qquad \mathbf{K}(\boldsymbol{\rho})\mathbf{u} = \mathbf{f}; \qquad V = V_0 \qquad 0 < \rho_{\min} \leq \rho \leq 1 \tag{1}$$

where u_{out} is the displacement at the output port, $\mathbf{K}$ is the structural stiffness matrix, $\mathbf{u}$ is the structural displacement vector, $\mathbf{f}$ is the applied load vector, V is the structural volume, V_0

is the objective structural volume, $\boldsymbol{\rho}$ is the design variables vector and $\rho_{\min}$ is the minimum value of the relative density.

3 Application Example

The example corresponds to an inverter mechanism with null displacements in the upper and the lower part of the left edge. An horizontal force is applied in the input port (A) to maximize the horizontal displacement in the output port (B). Figure 1 shows the dimensions of the domain and the position of the input and output ports. Figures 2 and 3 show the optimal solution to the problem with the FEM-based and IGA-based formulation, respectively.

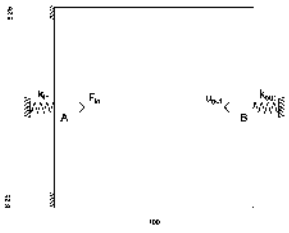


Figure 1: Domain Definition

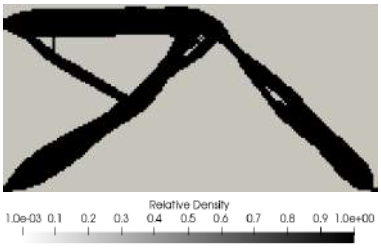


Figure 2: FEM-based solution

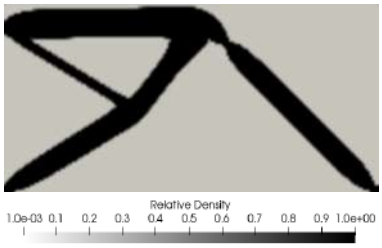


Figure 3: IGA-based solution

4 Conclusions

The IGA-based formulation proposed in this research to solve the topology optimization problem of compliant mechanisms provides solutions topologically equivalent to the classical FEM-based formulations. However, the spatial definition of the solution and the definition of its contour is improved. Moreover, the mesh dependence phenomena is mitigated.

5 Acknowledgements

This work has been partially supported by Spanish Government "(Ministerio de Universidades)" through "Margarita Salas grants for the training of new PhD - 2022" [RSU.UDC.MS25].

References

[1] Sigmund O. On the design of compliant mechanisms using topology optimization. J Str Mech 1997;25:493-524.

[2] Nishiwaki S, Frecker MI, Min S, Kikuchi N. Topology optimization of compliant mechanisms using the homogenization method. Int J Num Meth Eng 1998;42:535-559.

[3] Seao YD, Kim HJ, Youn SK. Shape optimization and its extension to topological design based on isogeometric analysis. Int J Sol Struc 2010;47:1618-1640.

[4] Kumar AV, Pathasarathy A. Topology optimization using B-splines finite elements. Str Mult Optim 2011;44:471-481.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Higher Order 3D-Shell Elements in Sheet Metal Forming Simulations: A Case Study

Maximilian Schilling*, Tobias Willmann* and Manfred Bischoff*

* Institute for Structural Mechanics
Faculty of Civil and Environmental Engineering, University of Stuttgart
Stuttgart, Germany
e-mail: {schilling, willmann, bischoff}@ibb.uni-stuttgart.de

Abstract: Most sheet metal forming simulations employ Reissner-Mindlin shell elements. The assumptions for these elements include that there is no transverse normal stress and that the material fibers remain straight during deformation. In some cases, such as bending with small radii, this approach is not sufficiently accurate because the cross-sections may become distorted and the strain distribution in the thickness direction may be highly nonlinear (Fleischer, 2009). To improve the accuracy of these simulations, Willmann et. al. (2021) introduced a higher order 3D-shell element, which can account for these effects.

In order to establish a priori guidelines for the efficient utilization of this higher order 3D-shell element in sheet metal forming simulations, we conduct a study of the magnitude of the higher order deformations for benchmark problems. By analyzing the magnitude of the higher order degrees of freedom and their change for parameter alterations, we can identify the situations under which the additional deformation modes of this element are beneficial for accurately modeling sheet metal forming processes.

Keywords: Higher order 3D-shell elements, sheet metal forming, applications

1 Introduction

In certain sheet metal forming simulations, such as forming of thick sheets, Reissner-Mindlin shell elements may not provide accurate results due to a violation of the underlying assumptions [1]. To improve the accuracy of these simulations, Willmann et. al. [2] developed a higher order 3D-shell element, which can model cross-sectional warping and a higher order strain distribution with respect to the sheet thickness coordinate. Various components of deformation of this element are depicted in Figure 1, further details can be found in [2].

2 Evaluation of Numerical Studies

In this contribution, we analyze the magnitude of the higher order degrees of freedom (HO-DOFs) for a higher order 3D-shell element with respect to various parameters. First, we examine the deformation of a cantilever beam under a concentrated, increasing moment at the free end. The beam is discretized with ten rectangular elements, a linear elastic material is used. Figure 2 (left) shows the deformed configurations of the beam. We study this problem for different beam slenderness ratios ($\lambda = \frac{l}{t}$). Figure 2 (middle) plots the magnitude of the HO-DOFs, i. e. the higher order deformations at state 4, divided by the

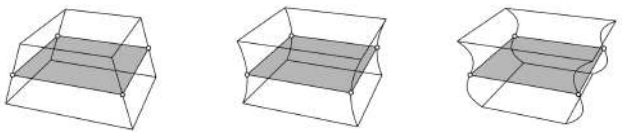


Figure 1: Deformation modes of the higher order shell element, including linear, quadratic, and cubic deformations of the cross-sectional fibers.

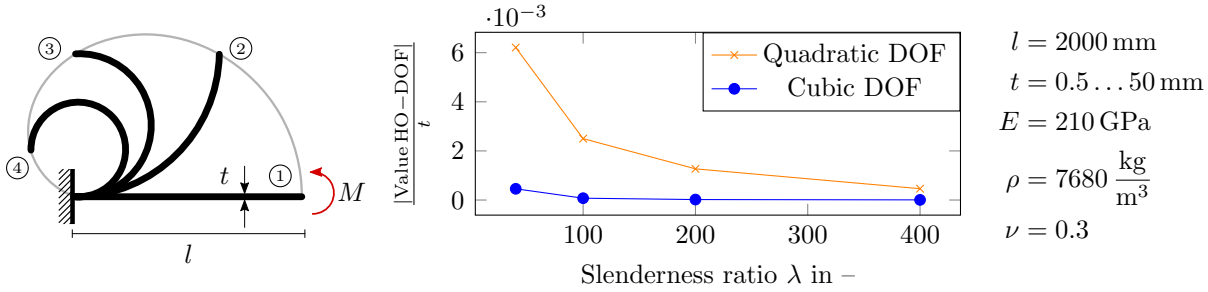


Figure 2: Cantilever beam under a concentrated moment at the free end (left), magnitude of the higher order degrees of freedom over element slenderness ratio (middle), parameters (right).

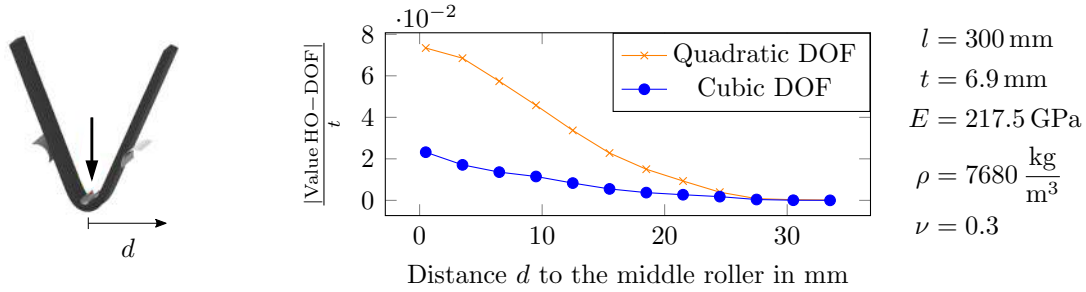


Figure 3: Three-point bending test (left), magnitude of the higher order degrees of freedom over distance to the middle roller (middle), parameters (right).

beam thickness t over the slenderness. The plot indicates that the ratio of the HO-DOFs relative to the beam thickness increases significantly for a slenderness greater than 200.

One example for a critical forming process is a three-point bending test of a flat sheet of thick metal (length l, thickness t). The middle roller is displaced, the two outer rollers are fixed. Figure 3 (left) shows the deformed configuration. An elasto-plastic material law is used. Figure 3 (middle) plots the magnitude of the HO-DOFs over the distance d to the middle roller. The graph indicates that the higher order deformations are localized around the middle roller and decay to zero within a distance of five times the sheet thickness.

3 Conclusions

Increasing the bending radius and slenderness ratio decreases the influence of the higher order deformations. Furthermore, this influence is limited to specific regions of a model. This suggests to use higher order 3D-shell elements only when they are beneficial for accurately modeling a sheet metal forming process. Further research on the influence of the HO-DOFs on quantities of interest, like strain, is needed. The project was funded by the German Ministry for Economic Affairs and Climate Action based on a decision of the German Bundestag as IGF project 21466 N. This support is gratefully acknowledged.

References

[1] Fleischer M. Absicherung der virtuellen Prozesskette für Folgeoperationen in der Umformtechnik. Thesis, Technical University of Munich; 2009.

[2] Willmann T, Wessel A, Beier T, Butz A, Bischoff M. Cross-Sectional Warping in Sheet Metal Forming Simulations. 13th European LS-DYNA Conference; 2021.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

3D ultrasonic tomography for image reconstruction: an application to the plasma dynamics of PROTOSPHERA

Naghinajad Shayesteh*, Pau Annamaria†

* Department of Astronautical, Electrical and Energy Engineering
School of Civil and Industrial Engineering, Sapienza University of Rome
Roma, Italy
e-mail: shayesteh.naghinajadmohammadkhanlou@uniroma1.it

† Department of Structural and Geotechnical Engineering
School of Civil and Industrial Engineering, Sapienza University of Rome
Roma, Italy
e-mail: annamaria.pau@uniroma1.it

Abstract:

A typical approach to 3D image reconstruction is computed tomography, which reconstructs the sought image based on a set of slice projections, relying on the Fourier slice theorem in 2D. We propose an imaging technique based on the Fourier slice theorem in 3D, which relates a set of projections onto planes, that is a 3D Radon transform, to a 3D Fourier transform. By calculating the 3D inverse Fourier transform, we can reconstruct the 3D image of the scanned object. The proposed formulation enabled us to reconstruct the distribution of magnetically confined plasma fed by electrodes in a cylindrical vacuum vessel.

Keywords: 3D Image reconstruction, Radon transform, ultrasonic tomography, plasma dynamics, inverse problems

1 Introduction

The classical approach in computed tomography consists in obtaining a 3D image based on a set of projections slices. A projection slice collects the integral of some measurable response quantity throught a set of plane (slice) parallel rays illuminating the object of interest. A review of the different approaches to image reconstruction can be found in [1]. A collection of parallel projections through an object onto lines at varying angles is called direct 2D Radon transform [2].The Fourier slice theorem guarantees that the Fourier transform of the Radon transform at a given angle equals the values of one row of the 2D Fourier transform. Then, the image is obtained by calculating the 2D inverse Fourier transform of the Radon Transform. In this way, a 3D image is obtained assembling the image of each slice.

Differently from that, in this work, we approach the solution to the inverse problem of 3D image reconstruction relying on the Fourier slice theorem in higher dimensions, that is in 3D. This approach is particularly useful when using a set of camera pictures, which are in themselves a discrete 3D Radon transform. We apply the algorithm proposed to the reconstruction of the spatial distribution of magnetically confined Hydrogen plasma. Data was provided by ENEA within the framework of the PROTOSHPERA project [3], which employs a spherical torus where a Hydrogen plasma arc, in a form of a screw pinch, fed by electrodes, replaces the central rod of the standard spherical torus experiments. During the experiment, the plasma emits photons, which are captured by six cameras arranged

with cylindrical symmetry. The accurate study of laboratory plasma dynamics with optic tomography could either provide useful information on the dynamics of plasma confinement, and on some astrophysical systems, where, though at a completely different scale, similar phenomena occur.

2 3D Radon transform

The extension of the Fourier slice theorem to higher dimensions, in particular to 3D, enables direct reconstruction of 3D objects employing a 3D Radon transform, that are sets of 1D projections or parallel line integrals of a function $f(x, y, z)$ representing the object, onto planes spanning all the possible normals in 3D [4]. The Fourier slice theorem in 3D guarantees that the image itself is the inverse 3D Fourier transform of this 3D Radon transform. In this work, the images captured by a set of cameras play the role of a discrete 3D Radon transform. The effectiveness of the procedure is displayed in Figure 1, which reports the six pictures captured by six cameras with cylindrical symmetry (a) and the related 3D reconstruction of the distribution of plasma (b) in one time instant. Similar pictures are obtained in other time instants and reported in Figure 1 (c).

3 Conclusions

We have summarized an approach to computed tomography that employs the extension of the Fourier slice theorem to 3D. We have displayed that six pictures captured by cameras arranged in cylindrical symmetry enable a meaningful 3D reconstruction of the plasma spatial distribution in the PROTOSPHERA experiment at different time instants.

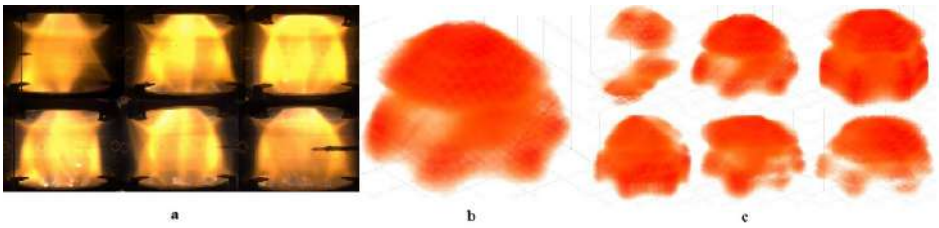


Figure 1: a) Pictures recorded by the six cameras at a given time instant of the PROTOSPHERA experiment and b) 3D reconstruction of plasma distribution c) reconstruction at different time instants

References

[1] Khairi MTM, Ibrahim S, Yunus MAM, Faramarzi M, Sean GP, Pusppanathan J, Abid A. Ultrasound computed tomography for material inspection: Principles, design and applications. Measurement 2019;146:490-523.

[2] Kak AC, Slaney M. Principles of computerized tomographic imaging. Society for Industrial and Applied Mathematics; 2001.

[3] Alladio F, Costa P, Mancuso A, Micozzi P, Papastergiou S, Rogier F. Design of the PROTO-SPHERA experiment and of its first step (MULTI-PINCH) Nucl. Fus. 46, S613; 2006.

[4] Averbuch A, Shkolnisky Y. 3D Fourier based discrete Radon transform. Appl. Comput. Harmon. Anal. 2003; 5: 33–69.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Application of LCA modelling methods as a tool to identify hotspots in the development of metal recycling processes

Katarzyna Klejnowska[*], Magdalena Bogacka[†]

[*] Department of Metallurgy
Łukasiewicz Research Network – Institute of Non-Ferrous Metals
Ul. Sowińskiego 5, 44-100 Gliwice
e-mail: katarzyna.klejnowska@imn.lukasiewicz.gpv.pl

[†] Department of Technologies and Installations for Waste Management
Faculty of Energy and Environmental Engineering
Silesian University of Technology
Ul. Konarskiego 18, 44-100 Gliwice
e-mail: magdalena.bogacka@polsl.pl

Abstract: European Green Deal and the resource independence from the non-EU countries require the development of modern and flexible solutions allowing to process different types of waste and re-cover as much secondary resources as possible. Life cycle assessment (LCA) is a tool that can be used identify and quantify the environmental effects and hotspots of products or processes in their whole life cycle, including mining, processing, manufacturing, transportation, distribution, utilization and recycling. The implementation of an LCA-based study can be a powerful tool when applied during the development of new technologies and can contribute to the improvement of the existing processes, as it provides a multi-disciplinary overview on the most important environmental loads associated with the developed recycling technologies. The presentation will be focused on the application of LCA methods to identify and minimize the negative impact of the recycling technologies.

Application of process simulation software to design of hydrometallurgical process of germanium recovery

Michał Drzazga

Centre of Hydroelectrometallurgy
Lukasiewicz Research Network – Institute of Non-Ferrous Metals
Gliwice, Poland
e-mail: michal.drzazga@imn.lukasiewicz.gov.pl

Abstract: Application of HSC Chemistry 9 software to design of hydrometallurgical process of germanium recovery is presented. Flowsheet simulation module *SIM* was applied for the design of preliminary technological flowsheet. The technology is composed of two main parts. The first one is leaching of copper-cobalt cake containing ca. 200 ppm germanium as well other component like zinc, copper, cadmium, nickel, cobalt, lead followed by subsequent precipitation with tannic acid to get germanium-tannin preconcentrate. In the second one preconcentrate is further processed to obtain final product – germanium concentrate containing >10% germanium. The aim of the study is to design technological process consisting of the sequence of unit operations and use HSC Sim software to further develop the process as well as to calculate mass balances. Final results will be the base for further development of the process during piloting stage as well as during calculation of process costs and design of the final industrial installation.

Keywords: germanium, process development, leaching, precipitation, HSC Chemistry

1. Introduction

HSC Chemistry is a software toolkit developed originally by company Outotec, which is now known as Metso Outotec. Its primary purpose is to perform calculation of chemical reactions and equilibria using built in database as well as user data. The software consists of several different modules like: Reaction Equations, Heat and Material Balances, Equilibrium Compositions, H, S, Cp Estimates, which might be useful at different stages of chemical operation design. One of the modules - Flowsheet Simulation (*Sim*) - may be used the design of the whole chemical process as it allows to combine calculation of several unit operation in one technological cycle. This module allows design of the almost whole metallurgical process – from mineral processing stage to final products, including also pyrometallurgical and hydrometallurgical operations as well as phase separation units.

2. Description of the process

Designed process is composed of the series of unit operation. Technological scheme is presented in Figure 1. In the first stage copper-cobalt cake (composition provided in Table 1) is leached under non-oxidative conditions in 15 wt.% aqueous solution of sulfuric acid. Then, suspension is filtered using pressure filter press. The cake is also washed with water. Filtrate then may be used for recovery of cadmium, zinc, nickel and cobalt, while the solid phase is directed to the second stage of the process, where it is subjected to oxidative leaching (using air) in 12.5 wt. % aqueous solution of sulfuric acid. Obtained suspension is

Table 1. Composition of the copper -cobalt cake

Element	Cu	Cd	Zn	Pb	Ni	Co	Ge	Moisture
Content [wt.%]	24.7	21.2	16.3	4.50	3.96	3.22	231 ppm	38.7

filtered. Cake after the 2nd stage may be used for lead recovery, while solution is directed to the next stage in which germanium is precipitated from solution using tannic acid. Suspension of germanium-tannin preconcentrate is filtered, while solution may be directed to copper recovery technology. Then, the preconcentrate is dried and combusted in air to obtain final germanium concentrate.

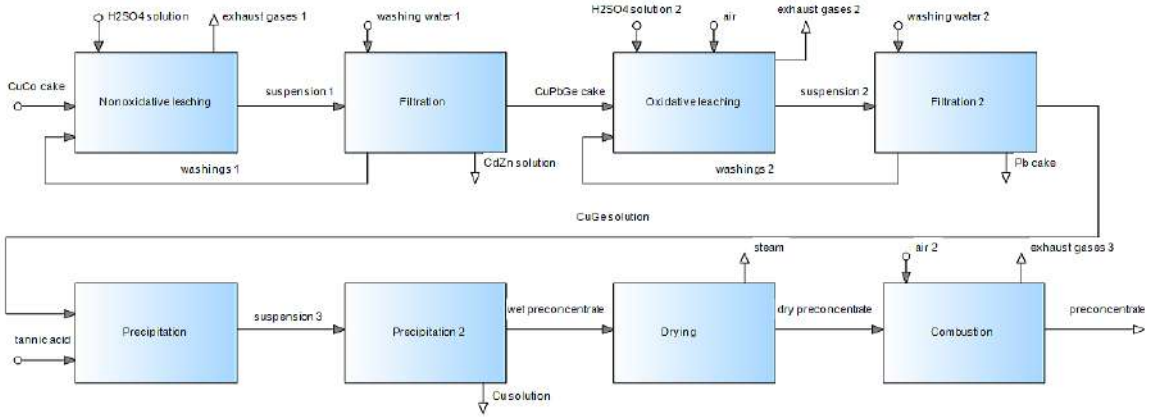


Figure 1 Scheme of simulated process prepared in HSC Chemistry 9 software (*Sim* module)

3. Process simulation

The aim of the study is to simulate design process based on obtained experimental results as well as on bult-in thermodynamic data and to compare experimental composition of streams with simulated ones (Table 2). Simulation was based on the presence of the following species in the process: H_2, O_2, N_2, H_2O and CO_2 in gas phase, H_2O, Cd^{2+}, Cu^{2+}, Zn^{2+}, Ni^{2+}, Co^{2+}, $Ge(OH)_4$, $HGeO_3^-$, H_2SO_4, SO_4^{2-}, H^+ in aqueous phase as well as $Cd(OH)_2$, Cu, Cu_2O, Zn, PbO, $CuSO_4 \cdot 5H_2O$, $CdSO_4 \cdot 2.667H_2O$, $ZnSO_4 \cdot 7H_2O$, $NiSO_4 \cdot 7H_2O$, $CoSO_4 \cdot 7H_2O$, Ge, GeO_2, $PbSO_4$, Co and Ni in solid phase.

Table 2. Composition of solid and aqueous phases based on experiments and simulation

Element	Cu	Cd	Zn	Pb	Ni	Co	Ge
			CuPbGe cake				
Experimental	57.5	2.50	3.24	9.70	2.15	1.73	420 ppm
Simulated	72.4	0.14	0.10	13.2	0.03	0.02	630 ppm
			Pb cake				
Experimental	2.60	1.86	2.57	33.3	0.05	0.01	410 ppm
Simulated	0.09	<0.01	<0.01	60.7	<0.01	<0.01	623 ppm

Preliminary results indicates that there are quite significant differences between experimental results and simulated ones. Simulated results are based only on thermodynamic calculations and does not include effects associated with reaction kinetics or occlusions.

Acknowledgements

This activity has received funding from the National Centre for Research and Development within LIDER XI programme (grant no. 43/0159/L11/19/NCBR/2020) “Innovative technology for germanium recovery from wastes of Polish zinc metallurgy”.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Investigations on the Detection of Structural Failure Using the Redundancy Distribution

Tamara Prokosch*, Jonas Stiefelmaier†, Manfred Bischoff*

* Institute for Structural Mechanics
Faculty of Civil and Environmental Engineering, University of Stuttgart
Stuttgart, Germany
e-mail: prokosch@ibb.uni-stuttgart.de

† Institute for System Dynamics
Faculty of Engineering Design, Production Engineering and Automotive Engineering, University of Stuttgart
Stuttgart, Germany

Abstract: Adaptive structures can reduce the use of material by changing their shape and redistribute stresses. They are equipped with sensors and actuators to do so and the most recent research is focusing on their design and performance.
The redundancy distribution, based on the concept of static indeterminacy, provides insight into the load-bearing behavior of structures. It can be used to describe the effects that changes in topology and materiality have on stresses from constraint and resulting deformations in structures. Making use of the properties of both redundancy distribution as well as adaptive structures, methods to detect and identify structural failure are examined by analyzing a series of varying structures and possible failure modes. Special focus is given to the localization of the failure and its extent. In conclusion of the results, early detection of structural failure in adaptive structures can be an opportunity for timely and targeted reaction and therefore, safer and more reliable structures.

Keywords: structural failure, failure detection, adaptive structures, redundancy

1 Introduction

Adaptive structures are an advanced technology using sensors and actuators to change shape and redistribute stresses, reducing the mass required for the structure and ultimately saving costs and resources. However, as with any new technology, safety considerations are important, particularly when it comes to structural failure. The sensors and actuators in adaptive structures offer a unique opportunity to monitor structural health and detect potential failure at an early stage, allowing for timely repair and support measures.

2 Methods

The redundancy matrix, as proposed by Bahndorf [1] and derived for frame structures by von Scheven [2], is a system describing matrix that provides information about the redundancy distribution in a structure and thus on the contribution of each individual structural element to its static indeterminacy. By quantifying the constraint on each element exerted by the surrounding structure, the redundancy matrix grants insight into the load-bearing behavior

of the structure. Thus, Chen et al. [3] proposed the application of the matrix for load path analysis and derived a formula for updating the redundancy matrix in case of member loss. This lays the foundation for investigations on the detection of structural failure of elements and changes in element properties due to changes in the redundancy distribution.

3 Numerical Examples

A study is conducted on various systems, with different topologies and materials. Structural analysis and the implementation of the redundancy distribution are carried out both for the original systems, as well as for variants with missing or damaged elements. Aiming for detectability measures, changes in stress distribution and deformations for general load cases and changes in the redundancy distribution of the system are analyzed. In addition, methods utilizing the properties of adaptive structures are tested to assess the effectiveness of detecting and identifying structural failure.

4 Conclusions

The results imply that the redundncy matrix is a promising tool for detection and identification of structural failure in adaptive structures. Early identification of damage provides the opportunity for instant counter-action. This method has the potential to raise the level of safety in adaptive structures. Further research on this topic is needed to validate and optimize the proposed methods.

5 Acknowledgements

This work is conducted in the framework of the Collaborative Research Centre 1244 funded by the Deutsche Forschungsgemeinschaft (DFG - German Research Foundation).The authors are grateful for the generous support.

References

[1] Bahndorf, J., 1991. Zur Systematisierung der Seilnetzberechnung und zur Optimierung von Seilnetzen, Deutsche Geodätische Kommission bei der Bayerischen Akademie der Wissenschaften Reihe C, Dissertationen. Verlag der Bayerischen Akademie der Wissenschaften, München.

[2] von Scheven, M., Ramm, E., Bischoff, M., 2021. Quantification of the redundancy distribution in truss and beam structures. International Journal of Solids and Structures 213, 41–49.

[3] Chen, Q., Kou, X., Zhang, Y., 2010. Internal force and deformation matrixes and their applications in load path. J. Zhejiang Univ. Sci. A 11, 563–570.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Cost Reduction of Water Supply Systems Through Optimization Methodologies: A Comparative Study of Pump Scheduling Problem Formulations

Marlene Brás*, Ana Moura* and António Andrade-Campos†

* Department of Economics, Management, Industrial Engineering and Tourism
University of Aveiro
Aveiro, Portugal
e-mail: {marlenegomes, ana.moura}@ua.pt

† Department of Mechanical Engineering, Centre for Mechanical Technology and Automation
University of Aveiro
Aveiro, Portugal
e-mail: gilac@ua.pt

Abstract: The global water supply represents 7% of the global energy consumption. Considering the evolution of the energy tariffs, reducing the energy consumption of water supply systems (WSS) has never had a more significant impact. From the three main operating areas in WSS, the pump operation is the most critical one, since 70% of the energy consumption in WSS is represented by the energy consumed in pumping stations due to water pumping. This high energy consumption makes pumping stations' energy efficiency a critical factor in terms of the sustainability of water management entities, promoting the adoption of smart solutions capable of reducing costs. The efficiency of the pump operation can be improved directly through the mathematical formulation of the pump scheduling problem and there are several mathematical formulations for this optimization problem. However, there are no comparative studies between them, and since each WSS system has different physical characteristics, each formulation may result in a different performance for the same WSS. As a consequence, it is still an open question which formulation is the most efficient and robust for this particular problem. This work aims to present a comparative study of the three WSS problem formulations.

Keywords: Pump Scheduling, Optimization Models, Water Supply Systems

1 Introduction

A water supply system (WSS) is a vital infrastructure that transports water from sources to consumers in the required quantity and pressure [1]. It plays a crucial role in urban areas, with the primary goal of delivering clean drinking water from water treatment plants to end-users [2].

Energy efficiency in WSS is crucial for the sustainability of water management entities and requires the implementation of smart solutions to reduce costs. As these costs continue to rise faster than inflation, managing energy operations becomes increasingly complex and cannot be solely reliant on the know-how of experienced employees. The operation of WSS is typically guided by operating rules that balance competing objectives such as minimizing operational costs, energy use, and flood risk while maintaining water quality. In terms of energy costs, the pump operation of pumping stations is the most critical aspect, since it

represents 70% of the WSS energy consumption. Historically, the optimal pump scheduling problem has been formulated as an implicit control problem or as an explicit control problem. In the implicit formulations, the decision variables relate to system characteristics that are controlled by external stimuli, such as pump flows, pressure, water tank levels. In contrast, in explicit formulations, pumps are directly controlled through its scheduling and the decision variables are related to pumps' operation times. This formulation type can be further divided into two categories: time-position-restricted and time-position-unrestricted. In all formulations for this optimization problem, the objective is to minimize the cost of energy consumed by pumps during the total time horizon, which is typically 24h. There are several constraints that could be considered, including maintaining minimum and maximum water levels in tanks, limiting the number of pump startings during the total time horizon, conservation of the system's mass and energy in terms of flow q, ensuring minimum pressures, etc. Although there are several mathematical formulations for this optimization problem, there are no comparative studies between them.

2 Aim

This work's objective is to quantitatively compare three explicit formulations, being them two time-position-restricted and one time-position-unrestricted. Three case studies were implemented and the key performance indicators (KPIs) used to evaluate each formulation performance include the number of decision variables, processing time, number of objective function evaluations, and objective function value.

3 Acknowledgements

This work was supported by the doctoral grant (Ref. 2022.12310.BD) financed by the Portuguese Foundation for Science and Technology (FCT) and by the Regional Operational Program of the Center Region (CENTRO2020) within project I-RETIS-WATER (CENTRO-01-0247-FEDER-069857), through the COMPETE 2020 Programs.

References

[1] M. Manteigas, A. Andrade-Campos, A. Antunes, B. Coelho. Cost-Efficient Algorithms for a Pump Horizon Control in Water Supply System. Journal of Water Resources Planning and Management, 2022;148(1):1–15.

[2] P. T. Fracasso, F. S. Barnes, A. Helen, R. Costa. Energy Cost Optimization in Water Distribution Systems using Markov Decision Processes. International Green Computing Conference Proceedings, 2013.

[3] O. M. Awe, S. T. A. Okolie, O. S. I.Fayomi. Optimization of Water Distribution Systems: A Review. Journal of Physics: Conference Series, 2019;1378(2).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Energy storage using a hydraulic system a pump storage computacional model

Flávio Silva, António Andrade-Campos

* Department of Mechanical Engineering
Centre for Mechanical Technology & Automation University of Aveiro
Aveiro, Portugal
e-mail: flaviosilva99@gmail.com

Abstract: Environmental sustainability has been increasingly present in our daily lives. Over the years, the environmental impact caused by anthropogenic sources such as the use of fossil fuels in the production of electricity has had devastating consequences for nature and for human beings. However, today it is possible to observe a paradigm shift in electrical energy production. Investments in renewable energy sources such as solar, wind, geothermal or hydroelectric power are increasingly a clean and viable alternative.
However, the need to store large amounts of energy in periods of energy availability and recover it in periods of energy consumption is still a problem. New storage technologies are often impractical in aspects such as the amount of energy, durability, and efficiency, making them unprofitable. With this, energy type conversion technologies, for example, pump storage, which accumulates gravitational potential energy by converting it into electrical energy can be a solution. The objective of this work is to create a parameterized computacional model of Pump Storage technology in order to controlate to the amount of energy to be collected, its efficiency, and the availability of energy and taking to account the price of electricity in the market as well.

Keywords: Energy, Pump storage, hydroelectric, energy tariffs, computacional model

1. Introduction

In recent years, measures aimed at the development of clean technologies have been a strong bet for the decarbonization of the energy sector, diversification of electricity production, and a reduction in foreign energy imports, improving national energy security. However, the biggest problem with the production of renewable energy is its high intermittency. Natural energy conversion technologies for electrical energy production such as wind turbines or photovoltaic panels are dependent on their primary energy, wind, and solar radiation, respectively, which limit continuous production for long periods. Thus, rather than installing more renewable energy, it is essential to look for ways and alternatives to store that energy. Pump storage technology is a water storage technology between two reservoirs, with different levels, which storage gravitational potential energy and, when necessary, converts it into electrical energy.

2. Extended abstract content

This work aims to develop an energy storage model using a hydraulic system: Pump Storage. The computacional model in question has the primary characteristic of being a parameterized model, representing any operating situation. The aim is thus to evaluate the operating scenarios whether on a small scale or in a more urbanistic aspect and analize their sensitivity to different storage values. A study is also carried out on the complementarity of this system and for several different daily energy markets, maximizing gains from the difference in purchase and sale prices of energy.

4. Conclusions

The model developed estimates the sensitivity of a pump storage system in different scenarios. Predictably, its viability is proportional to the size of the system, that is, larger the storage capacity, larger the energy, and its financial return. Regarding profit maximization, the model is able to assess the complementarity between market energy prices and the need to recover energy to determine its operating range.

Acknowledgements

The authors gratefully acknowledge the financial support of the Portuguese Foundation for Science and Technology (FCT) and UE/FEDER through the programs CENTRO 2020 and COMPETE 2020 and UID/EMS/00481/2013-FCT under CENTRO-01-0145- FEDER-022083 and Programa Operacional Regional do Centro, through the project I-RETIS-WATER (CENTRO-01-0247-FEDER-069857).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A Mixed-Integer Nonlinear Programming Model for Integrated Management of Resources in Water Supply Systems

Ana L. Reis[*†], A. Andrade-Campos[†], Carlos Henggeler Antunes[*] and Marta A. R. Lopes[*+]

[*] INESC Coimbra
Department of Electrical and Computer Engineering, Polo II, University of Coimbra,
Coimbra, Portugal
e-mail: uc2020153533@student.uc.pt

[†] Department of Mechanical Engineering, Centre for Mechanical Technology & Automation
University of Aveiro
Aveiro, Portugal

[+] Polytechnic Institute of Coimbra, Coimbra Agriculture School,
Bencanta, 3045-601
Coimbra, Portugal

Abstract: Water supply systems (WSS) are energy intensive infrastructures encompassing water storage tanks and pumping systems to deliver water to consumers. Due to the current challenges facing the water sector, especially the rising of energy prices, improving the operational efficiency of WSS is paramount. Water utilities that are willing to participate in demand-side management programs can reduce their energy costs by implementing cost-effective load management strategies. These strategies include shifting the operation of pumping loads when time-differentiated energy prices are available, investing in on-site renewable energy generation and storage systems, such as batteries, while satisfying the consumers' demand. Since the WSS operational decision process must be fast and dynamic, in some cases almost near real-time, the successful implementation of these strategies calls for appropriate tools to support decision making. Therefore, the aim of this work is to develop a mixed-integer nonlinear programming (MINLP) model addressing in a comprehensive manner the demand side flexibility of WSS operation by making the most of the integrated resources management (e.g., water quantity, local renewable generation, shiftable pumping loads, water storage tanks, energy bought from the grid considering time-differentiated energy prices and storage systems) to reduce energy costs. Computational results on a case study are presented, showing the effectiveness of the proposed approach.

Keywords: Water supply systems, demand-side management, integrated management of resources, mixed-integer nonlinear programming model, load management strategies.

1 Acknowledgements

This research was supported by the doctoral Grant SFRH/BD/151347/2021 financed by the Portuguese Foundation for Science and Technology (FCT) under MIT Portugal Program and through the Regional Operational Program of the Center Region (CENTRO2020) within project I-RETIS-WATER (CENTRO-01-0247-FEDER-069857), UIDB/00481/2020 and UIDB/00308/2020 through the European Social Fund, European Regional Development Fund and the COMPETE 2020 Programs and the Energy for Sustainability Initiative of the University of Coimbra.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

On the use of Machine Learning models for prediction and optimization of water supply networks.

Sara Mota[*], **António Andrade-Campos**[†]

[*] Department of Environment and Planning (DAO)
Universidade de Aveiro
Aveiro, Portugal
e-mail: saramota@ua.pt

[†] Department of Mechanical Engineering (DEM), TEMA research unit
Universidade de Aveiro
Aveiro, Portugal
e-mail: gilac@ua.pt

Abstract: With the continuous increase of energy prices, the nexus water-energy needs a solution for the efficiency increasing of water distribution systems. Decision support systems and hydraulic simulators, such as EPANET, have proven to be a solution for several years. However, the experience has showed that these hydraulic models are too complex and require a high computational effort for both development and calibration. In order to mitigate this problem, Machine Learning (ML) have been used. In this study, supervised learning ML models are analyzed and compared to EPANET performance. It is expected to contribute with a faster, more accurate and with lower associated development costs model.

Keywords: Water distribution systems, energy, Machine Learning, modelling, optimization, pump scheduling.

1 Introduction

As society evolves through time, the use of resources increases. Water is the main resource indispensable for life, and its increasing demand has directly increased the energy usage for its distribution. Therefore, the need to efficiently distribute and manage these two resources is the foremost important goal of recent times. This need led to the development of decision support systems (DSS) to optimize water distribution, and hydraulic simulators as for example EPANET. These systems allow to model the real system and optimize it. However, these have limitations such as the complexity of calibration and the high computational effort, increasing the costs of the operation. To mitigate these disadvantages smart predictive control models have been developed recurring to advanced technologies such as Machine Learning algorithms to reach an optimal control of the water distribution. These models can learn from experience (data samples) and develop a prediction.

2 Methodology

In this work, different architectures of machine learning models are analyzed for their effectiveness in predicting and optimizing water distribution. Supervised learning models are used in three case studies. These models are trained and validated on data sets of historical

water usage patterns and evaluated based on their ability to make an accurate prediction when compared to EPANET. It is intended to also use energy price variation to optimize the pump control schedule, lowering the cost of the operation.

3 Conclusions

The expected conclusions of this study are of a fastest, more accurate, and less expensive model for the water distribution problem. These achievements are useful for water utilities and other stakeholders in the water industry, as they can use the insights from this study to choose the most appropriate solution for their specific needs. The study also contributes to the academic community with the use of machine learning in smart water systems and the development of more advanced and effective water distribution technologies.

4 Acknowledgements

The authors gratefully acknowledge the financial support of the Portuguese Foundation for Science and Technology (FCT) and UE/FEDER through the programs CENTRO 2020 and COMPETE 2020 and UID/EMS/00481/2013-FCT under CENTRO-01-0145- FEDER-022083 and Programa Operacional Regional do Centro, through the project I-RETIS-WATER (CENTRO-01-0247-FEDER-069857).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Smart predictive digital twin in multiservice architecture for water supply systems

Tiago C. Pereira [*], **Ana L. Reis** [*†], **António Andrade-Campos**[*]

[*] Department of Mechanical Engineering, Centre for Mechanical Technology & Automation
University of Aveiro,
Aveiro, Portugal
e-mail: tiago.crispim@ua.pt

[†] INESC Coimbra
Department of Electrical and Computer Engineering, Polo II, University of Coimbra,
Coimbra, Portugal

Abstract: Water supply systems (WSS) are essential infrastructures that ensures reliable and safe distribution of water. An important feature of these systems is the implementation of efficient pump scheduling operations that minimize energy costs, while respecting the network's constraints (e.g., water tank levels, minimum pressures). An optimal predictive control requires an accurate representation of the system, which can be achieved by using a digital replica (i.e., a digital twin) which allows simulating or forecasting the system's states. For an effective and efficient pump control, the system needs to be able to integrate data streams from several sources, such as sensors and prediction models, driving the design of service-based frameworks. The original contribution of this work is to present a multiservice framework that aggregates data from several sources, and a smart predictive digital twin for pump scheduling. The developed system assesses the performance of each service and its corresponding contribution to the overall system's performance.

Keywords: Digital Twins, Water Supply Systems, Forecasting, Multiservice Frameworks, Model Predictive Control, Machine Learning

1 Introduction

Recently, virtual representations of physical systems, commonly known as Digital Twins, have emerged as powerful tools in a multitude of disciplines that require emulation of complex real-world systems. In the field of Water Supply Systems (WSS) several studies have been made on the implementation of Digital twins, for example, for the prediction of infrastructure performance [1], water leakage control [2]. In regard to WSS, Digital Twins could be combined with optimal control techniques, such as model predictive control, for the execution of pump scheduling. Due to the nature of existing WSS, real-time processing is considered to be in the order of minutes, which makes model predictive control a suitable option. In addition to the control paradigm, WSS increase the complexity of the problem by the need of integrating multiple sources of information that need to be processed. SCADA or simlar technologies are often used for handling the streaming of data from several sensors throughout the water system network. Designing a framework that handles large amounts of information (big data), and ensures data interoperability, impacts factors such as scalability, observability, and cost, as discussed in [3]. In addition to sensor data, the system could incorporate data from prediction models, such as forecasts of water demand, energy cost,

and weather. This culminates in the design of multiservice frameworks, in which the system uses several modules that function independently, but work towards the same goals.

2 Proposed solution

This research presents a smart predictive digital twin integrated in a multiservice architecture that aggregates data from several sources (sensors and model outputs), and manages pump controls, minimizing costs. The proposed system is implemented in a real-time context and the predictive digital twin (which will be a machine learning model) is trained with simulated data (from EPANET software [4]) representing the real-world physical system. The system deploys models that predict water demand in each water junction, power cost, and the digital twin itself which uses the previous data to forecast tank levels, and energy used by pumps.

3 Conclusion

The developed multiservice system is capable of scheduling efficient pump controls that minimize energy costs, while respecting the WSS's constraints. Data management in services facilitates an independent evaluation of each model's performance. It also makes it possible to monitor the impact of each module on the overall system performance. This consequently helps in optimal resource and time allocation during development of each component.

4 Ackonwledgements

The authors gratefully acknowledge the financial support of the Portuguese Foundation for Science and Technology (FCT) and UE/FEDER through the programs CENTRO 2020 and COMPETE 2020 and UID/EMS/00481/2013-FCT under CENTRO-01-0145- FEDER-022083 and Programa Operacional Regional do Centro, through the project I-RETIS-WATER (CENTRO-01-0247-FEDER-069857).

References

[1] J. E. Pesantez, F. Alghamdi, S. Sabu, G. Mahinthakumar, and E. Z. Berglund, "Using a digital twin to explore water infrastructure impacts during the COVID-19 pandemic," Sustainable Cities and Society, vol. 77, p. 103520, Feb. 2022, doi: 10.1016/j.scs.2021.103520.

[2] H. M. Ramos et al., "New Challenges towards Smart Systems' Efficiency by Digital Twin in Water Distribution Networks," Water, vol. 14, no. 8, Apr. 2022, doi: 10.3390/w14081304.

[3] Carlos Manuel Basílio Oliveira. "Towards a scalable software Architecture for Water utilities' Decision Support Systems." Master's Dissertation, Universidade de Aveiro, Portugal, 2022.

[4] Rossman, Lewis A. EPANET Users Manual : Project Summary. Cincinnati, OH :U.S. Environmental Protection Agency, Risk Reduction Engineering Laboratory, 1994.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical and experimental characterization of 3D printed lattice structures

M. Carraturo*, G. Alaimo, A. Reali, F. Auricchio

Department of Civil Engineering and Architecture
University of Pavia
Via Ferrata 3, 27100, Pavia, Italy
e-mail: massimo.carraturo@unipv.it

Abstract: In this contribution, the complex process-structure-property-performance relationships occurring in octet lattice cell structures produced by means of laser-based powder bed fusion of metals are investigated. First, an empirical procedure suitable to define a SS 316L lattice material model is introduced and validated, then, an image-based numerical characterization of a 3D printed octet lattice cell is presented.

Keywords: Laser powder bed fusion, lattice structure, tensile test, numerical modeling, immersed boundary methods

1 Introduction

Numerical characterization of 3D printed lattice structure mechanical behavior is a challenging task due to the inhomogeneous material micro-structure and the complex geometry of these components. In the first part of the present contribution, an empirical, multi-scale procedure suitable to define a SS 316L lattice material model is presented and validated. In the second part, we address the geometrical issues of lattice components.

2 Methods and Contents

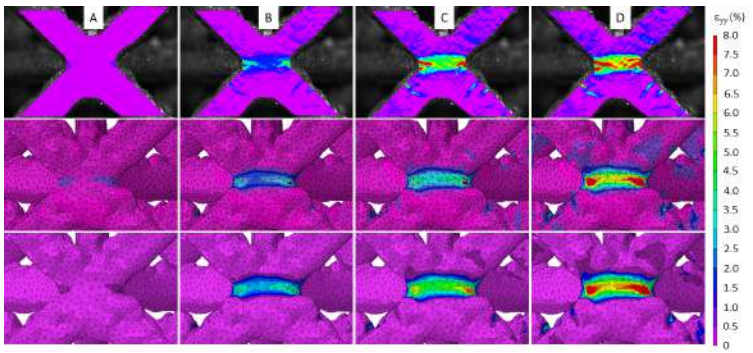


Figure 1: Experimental and numerical strain values comparison [1]

Multi-scale methodology for stress-strain response Starting from micro-indentation measurements, the yield stress and the Young modulus of the 3D printed material are obtained at nodal and truss locations on two different planes: the former parallel to the building direction and the latter perpendicular to the building plane. By means of an exponential

plastic law the micro-indentation measurements are used to define four isotropic material models. Experimental tensile tests were conducted using Digital Image Correlation (DIC) technique showing that the actual mechanical behavior of a lattice tensile specimen lies between the numerical curves [1] (see, fig. 1).

Image-based numerical characterization It is well known form the literature that the elastic behavior of lattice structures is dramatically underestimated when computed on the as-designed geometry. Therefore, the actual 3D printed geometry as acquired for instance by Computed Tomography (CT) scan has to be used for the analysis. However, such a geometry can be very challenging to mesh, thus an efficient immersed boundary method, namely the Finite Cell Method (FCM), has been employed to perform accurate numerical simulations of 3D printed lattice components [2] (see, fig. 2).

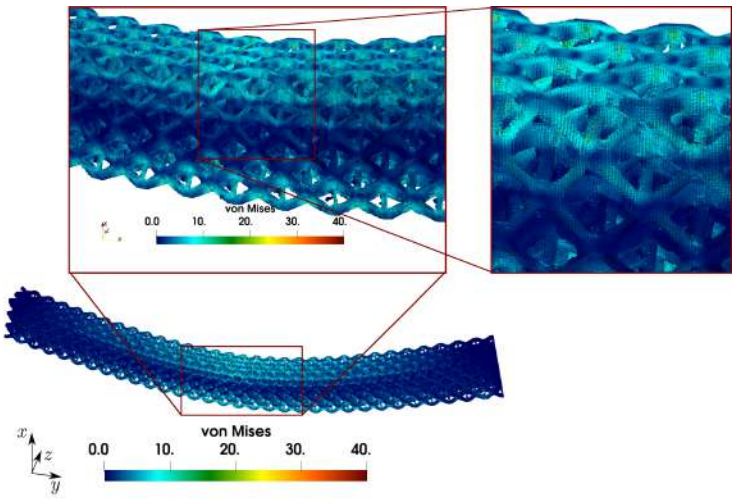


Figure 2: Von Mises stress distribution on a 3D printed octet lattice cell structure [2]

3 Conclusions

By exploiting different numerical and experimental approaches this work aims to shed lights on the complex process-structure-property-performance relationships occurring in octet lattice cell structures.

References

[1] Magarò P., Alaimo G., Carraturo M., Sgambitterra E., Maletta C., A novel methodology for the prediction of the stress-strain response of laser powder bed fusion lattice structure based on a multi-scale approach. *Material Science & Engineering A*, 2023.

[2] Korshunova N., Alaimo G., Hossein S.B., Carraturo M., *et al.*, Bending behavior of octet-truss lattice structures: Modelling options, numerical characterization and experimental validation. *Material & Design*, 2021.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Parametric shape optimization for combined additive-subtractive manufacturing

Lorenzo Tamellini*

* Istituto di Matematica Applicata e Tecnologie Informatiche
Consiglio Nazionale delle Ricerche
Pavia, Italy
e-mail: tamellini@imati.cnr.it

Abstract: In the industrial practice, additive manufacturing processes are often followed by post-processing operations such as heat treatment, subtractive machining, milling, etc. to achieve the desired surface quality and dimensional accuracy. Hence, a given part must be 3D-printed with extra material to enable such finishing phase. This combined additive/subtractive technique can be optimized to reduce manufacturing costs by saving printing time, reducing material and energy usage. In this work, a numerical methodology based on parametric shape optimization is proposed for optimizing the thickness of the extra material, allowing for minimal machining operations while ensuring the finishing requirements. The computational effort induced by classical constrained optimization methods is alleviated by replacing both the objective and constraint functions by their sparse-grid surrogates. Numerical results showcase the effectiveness of the proposed approach.

Keywords: Additive manufacturing, machining, parameteric shape optimization, constrained optimization, surrogate-based optimization, sparse grids

References

[1] L. Tamellini, M. Chiumenti, C. Altenhofen, M. Attene, O. Barrowclough, M. Livesu, F. Marini, M. Martinelli, and V. Skytt. Parametric Shape Optimization for Combined Additive–Subtractive Manufacturing. JOM - The Journal of The Minerals, Metals & Materials Society, 72:448–457, 2020

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Establishing and optimising structure-property linkages based on statistical descriptors

Raßloff, Alexander*; Seibert, Paul; Schmidt, Benjamin; Kalina, Karl A. and Kästner, Markus

Institut of Solid Mechanics, Technische Universität Dresden, Dresden, Germany
*e-mail: alexander.rassloff@tu-dresden.de

Additive manufacturing (AM) has a large potential but is still in the state of ongoing research and development as even small variations in the manufacturing process can have a significant impact on the resultant structure in terms of volume defects, surface characteristics or the microstructure. These, in turn, strongly influence the mechanical properties. This is why understanding the structure-property relationships is key for exploiting the full potential of AM [1].

In this contribution, we propose a general framework to computationally investigate the microstructure-property linkages. For deriving profound correlations, large databases are necessary. Experiments alone are prohibitively expensive. Therefore, computational augmentation is employed to allow for data-driven approaches. The general framework consists of four steps: (1) characterisation of microstructure images by translation-invariant descriptors by MCRpy [2], (2) reconstruction of three-dimensional microstructures from the descriptors by MCRpy [2], (3) numerical simulations to compute mechanical properties and (4) correlation of descriptors and properties and prediction/identification of descriptors of further microstructures for improved quality of the correlation. Step 2 is repeated.

This framework is applied and presented at the example of microstructure with hard precipitates of variable position and morphology in a softer matrix. For this purpose, a synthetic initial database of microstructures and corresponding properties is created using DREAM.3D [3]. Here, mechanical properties, such as yield strength, Young's modulus and fatigue indicator parameters are considered. Augmenting this small dataset by in silico reconstructed microstructures and their simulated properties allows for deriving improved structure-property linkages and, thus, predicting predicting properties or finding potentially optimal microstructures.

[1] A. Raßloff *et al.*, 'Accessing pore microstructure–property relationships for additively manufactured materials', *GAMM-Mitteilungen*, vol. 44, no. 4, 2021, doi: 10.1002/gamm.202100012.
[2] P. Seibert, A. Raßloff, K. A. Kalina, M. Ambati, and M. Kästner, 'Microstructure Characterization and Reconstruction in Python: MCRpy', *Integrating Materials and Manufacturing Innovation*, 2022.
[3] M. A. Groeber and M. A. Jackson, 'DREAM.3D: A Digital Representation Environment for the Analysis of Microstructure in 3D', *Integrating Materials*, vol. 3, no. 1, pp. 56–72, Dec. 2014, doi: 10.1186/2193-9772-3-5.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical and Experimental Investigation of Residual Stresses in the Fused Filament Fabrication Process

Lukhi Mehul, Mittermeier Christoph and Kiendl Josef

Institute of Engineering Mechanics and Structural Analysis
Faculty of Civil Engineering and Environmental Sciences, Bundeswehr University Munich
Munich, Germany
e-mail: mehul.lukhi@unibw.de

Abstract: In this study, the fused filament fabrication (FFF) process is modeled numerically to investigate residual stresses in the printed strand. In the FFF process, polymer filament is melted in the liquefier and molten polymer is extruded through the nozzle. The molten polymer flow is then deposited on the print bed with the nozzle traveling at a certain printing speed. In this study, the print bed is modeled as a rigid body that travels with prescribed print velocity, and the nozzle is kept stationary. For the modeling of the polymer flow through the nozzle, non-Newtonian and viscoelastic material models are used. To predict residual stresses in the printed strand, non-isothermal, thermo-mechanical flow simulations are performed. The free surface is resolved using the arbitrary Lagrangian-Eulerian (ALE) method. The effect of various printing process parameters such as nozzle temperature, bed temperature, printing speed, etc. on the residual stresses is investigated using simulations. The results obtained from the simulations are validated using experiments. The simulation results are in qualitative agreement with the experimental results.

Keywords: Fused filament fabrication, 3D printing, viscoelastic flow, residual stresses, arbitrary Lagrangian-Eulerian (ALE) method

1. INTRODUCTION

The FFF process is the most popular additive manufacturing process which is also popularly known as the 3D printing process. In this process, material in the form of either filament or granules is fed into the liquefier. The material is heated through the resistance heating and it melts down. The molten material extrudes through the nozzle and deposits on the print bed. Once the printing of the layer is completed, the print bed is lowered and another layer of printing begins. This is how layer by layer printing of the part is done.

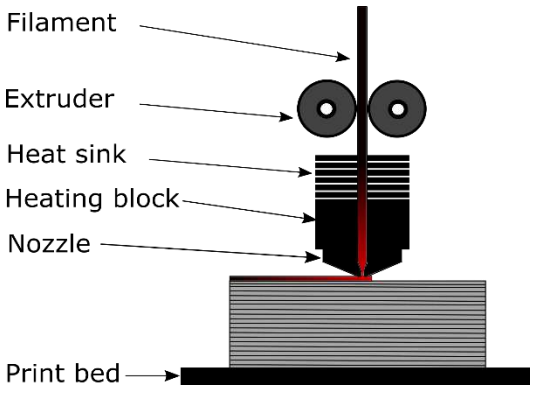


Figure 1 Schematic diagram of FFF process

Various researchers have performed fully-resolved simulations of the FFF process [1-3]. The residual stress prediction using a viscoelastic material model is not done in the literature so far. In this study, we aim to perform viscoelastic flow simulations to predict the residual stresses in the printed strand. In addition to that, we aim to perform a parametric study regarding the effect of various printing process parameters i.e. nozzle temperature, bed

temperature, printing speed, and cooling rate on the residual stresses. The simulation results are validated through the experiments.

2. Simulation Method

The simulation model for the molten polymer flow through the nozzle and deposition of the molten polymer flow on the print bed is shown in Fig. 2. For the modeling of the extrusion of the molten polymer, only the partial part of the nozzle which is filled with molten polymer is considered. The conical part of the nozzle is included because the molten polymer flow gets squeezed there and then it extrudes from the nozzle orifice. Appropriate flow and thermal boundary conditions are prescribed in the simulation model. The non-Newtonian and viscoelastic material models are considered in this study. The material parameters for the constitutive models are obtained using the rheological data available in the literature [4]. The print bed is modeled as a rigid body that travels with prescribed velocity. The free surface is resolved using the ALE method. The contacts between the free surface and the print bed, the free surface, and the external part of the nozzle are defined. For simulations, the commercially available Ansys Poly flow package is used. The residual stresses are extracted from the simulation results.

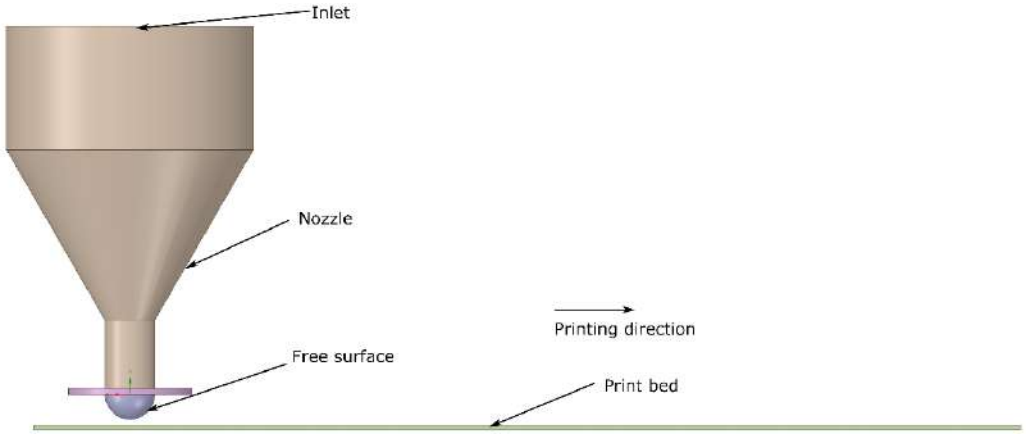


Figure 2 Simulation model of the FFF extrusion process

References

[1] A. Bellini, Fused deposition of ceramics: a comprehensive experimental, analytical and computational study of material behavior, fabrication process and equipment design. PhD thesis, Drexel University, 2002.

[2] M. Serdeczny, Numerical and Experimental Analysis of Filament-based Material Extrusion Additive Manufacturing. PhD thesis, Technical University of Denmark, 2020.

[3] H. Xia, J. Lu, and G. Tryggvason, A numerical study of the effect of viscoelastic stresses in fused filament fabrication, Computer Methods in Applied Mechanics and Engineering, vol. 346, pp. 242-259, 2019.

[4] S. Djellali, T. Sadoun, N. Haddaoui, and A. Bergeret, \Viscosity and viscoelasticity measurements of low density polyethylene/poly (lactic acid) blends," Polymer Bulletin, vol. 72, no. 5, pp. 1177-1195, 2015.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Application of Multi-fidelity Surrogate Models to Metal Additive Manufacturing

Mihaela Chiappetta[*], Chiara Piazzola[†], Massimo Carraturo[*], Lorenzo Tamellini[†], Alessandro Reali[*,†], Ferdinando Auricchio[*,†]

[*] Department of Civil Engineering and Architecture
University of Pavia, Via Ferrata 3, 27100, Pavia, Italy
e-mail: mihaela.chiappetta01@universitadipavia.it

[†] Istituto di Matematica Applicata e Tecnologie Informatiche "E. Magenes"
Consiglio Nazionale delle Ricerche, Via Ferrata, 5/A, 27100, Pavia, Italy

Abstract: The present work aims at applying uncertainty quantification methodologies to solve the limited knowledge of simulation parameters and mechanical behavior during additive manufacturing of metal components. To this end, we combine the computational efficiency of the sparse-grids matlab-kit algorithm with the performance of the Multi-Index Stochastic Collocation (MISC) method and build multi-fidelity surrogate models. In particular, we propose two MISC models to study uncertainties during the simulation of additive manufacturing with laser-based powder bed fusion technology of an Inconel 625 super-alloy beam.

Keywords: uncertainty quantification, additive manufacturing, Multi-Index Stochastic Collocation method, sparse-grids.

1 Introduction

In recent years, Additive Manufacturing (AM) for the production of metal components with complex geometries and remarkable mechanical performance has grown widely, with a market potential of several billion dollars. Among the various Metal AM technologies, the most popular are those based on powder bed fusion. In the present work, the focus is on the Laser-Based Powder Bed Fusion of Metals (PBF-LB/M) technology. In PBF-LB/M processes, metal powder particles are distributed on a build plate and selectively fused by a high-density laser source that follows a predefined scan path based on a 3D computer-aided design (CAD) model. Due to the inherent variability of process parameters (e.g., powder particle radius, mechanical properties of the powder particles, physical-chemical properties of the material), several sources of uncertainty hinder the knowledge of the variability of these processes. A key to addressing the above uncertainties is the adoption of Uncertainty Quantification (UQ) techniques during the AM process. The present work aims at applying UQ methodologies for the simulation of a PBF-LB/M process. For this purpose, we use Multi-Index Stochastic Collocation multi-fidelity surrogate models.

2 Multi-fidelity UQ methodology

The present work focuses on exploiting UQ techniques for accurate thermomechanical simulation of the PBF-LB/M process of an Inconel 625 beam (Figure 1). For this purpose, we take advantage of the computational efficiency of the sparse-grids matlab-kit algorithm and the

performance of the Multi-Index Stochastic Collocation (MISC) method to construct multi-fidelity surrogate models. In particular, we build a MISC model to calibrate and reduce the uncertainties of the activation temperature of the new layer and the powder convection coefficient, using an inverse Bayesian UQ approach. Afterwards, we use the calibrated and reduced parameters to build a second MISC model to accurately predict the residual strains of the beam, using a posterior-based forward UQ approach.

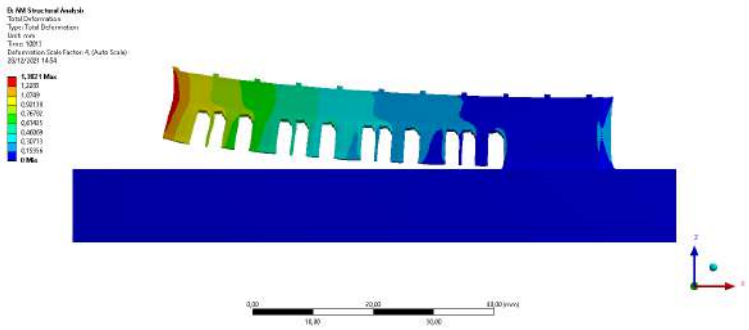


Figure 1: Inconel 625 beam model used for uncertainty quantification in PBF-LB/M simulations.

3 Results and Conclusions

We presents an inverse and forward UQ approach for accurate simulation of PBF-LB/M processes by studying the uncertainties involved. For this purpose, we use MISC multi-fidelity surrogate models that require lower computational cost than purely high-fidelity models. The results show that the application of inverse Bayesian UQ approach allows us to calibrate the activation temperature parameter and reduce the uncertainty of the powder convection coefficient. Based on these results, we show that with the posterior-based forward UQ approach, we are able to reduce the uncertainties in the prediction of residual strains by 98.3%. Furthermore, to computationally and experimentally validate our MISC models, we compare our results with those of the National Institute of Standards and Technology experiment.

References

[1] Carraturo, M., Jomo, J., Kollmannsberger, S., Reali, A., Auricchio, F., Rank, E. (2020). Modeling and experimental validation of an immersed thermo-mechanical part-scale analysis for laser powder bed fusion processes. Additive Manufacturing, 36, 101498.

[2] Piazzola, C., Tamellini, L., Pellegrini, R., Broglia, R., Serani, A., Diez, M. (2020). Uncertainty quantification of ship resistance via multi-index stochastic collocation and radial basis function surrogates: a comparison. In AIAA Aviation 2020 Forum (p. 3160).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical power prediction for WAM produced wall structures on vertical substrate plates

Haunreiter Fabio*, Drexler Hugo*, Kronsteiner Johannes* and Birgmann Alois*

* Austrian Institute of Technology (AIT)
Vienna, Austria
e-mail: fabio.haunreiter@ait.ac.at

Abstract: To enable a numerical WAM welding power prediction, a PID control function was combined with numerical welding simulations. This combination made it possible to adjust the welding power in order to reach a constant molten pool depth. The desired molten pool depth was experimentally determined. Based on a wall structure, the power prediction could be successfully tested.

Keywords: FEM, WAM, numerical welding power prediction

1 Introduction

Wire-Based Additive Manufacturing (WAM) enables the production of large near net shape component geometries. This makes WAM particularly interesting for industrial applications. The high heat input caused by the welding process, however, can lead to process instabilities. In order to avoid such instabilities, it is necessary to adapt the welding power to the current component temperature. This adaptation can be done in different ways. One attempt is to combine a control loop with FEM welding simulations. Numerical welding simulations can calculate the temperature field caused by the welding process. The control loop then uses the calculated maximum temperature from the simulation to adjust the welding power accordingly [1]. Besides the maximum temperature, it is also possible to use the width of the molten pool as an input for the control loop [2].

2 Method

This work is based on reference [3] and focuses on the implementation of a WAM-specific power prediction method in the FE-Software LS-DYNA. LS-DYNA provides a PIDCTL keyword which makes it possible to use a PID (proportional-integral-derivative) control loop function within the simulation software. External control tools, as they were used in [1] and [2] are no longer required. The calibration of the PIDCTL function was done based on experimentally determined results. In the experiments, a single seam was applied to a vertical aluminum substrate plate (Layer 1 in Figure 1 (b)). Therefore, a TIG welding process was used. The power of the welding process was varied until a visually good-looking seam was achieved. To ensure a valid calibration at different operating points the experiment was repeated at four different substrate preheating temperatures. In the end, the average penetration depth of the reference seams was 0.75mm. Seams welded with too much/too little power showed a higher/lower penetration depth. After the experiments, the welding process of one reference seam was simulated using LS-DYNA. Thereby, the parameters of

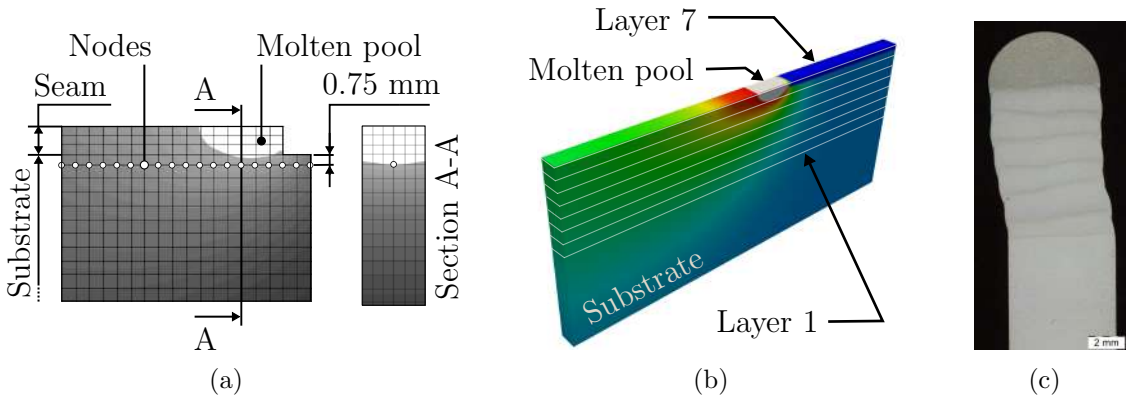


Figure 1: (a) Nodes temp. measurement (b) Contour plot wall (c) Micrograph wall

the PIDCTL function were adjusted so that a constant penetration depth of 0.75mm was achieved. This is made possible by the use of a temperature sensor in the simulation software. As schematically shown in Figure 1 (a), the sensor continuously measures the temperature of all nodes at a penetration depth of 0.75mm. In case the measured temperature deviates from the liquidus temperature of the material, the control function adjusts the power. This ensures a constant penetration depth of 0.75mm.

3 Validation

The calibration of the control loop was done based on a single seam on top of a vertical substrate plate. In the next step, the calibrated PIDCTL function was used to numerically predict the optimal welding power for six further seams (Figure 1 (b)). A cross section micrograph of the produced wall structure can be seen in Figure 1 (c). As required, the width of the welds corresponds to the width of the substrate plate. Thus, the welding power prediction led to the desired result.

4 Acknowledgements

The authors would like to thank the government of Upper Austria for sponsoring the research work in the project “PsHeRo:Er” (Wi-2020-700757/4-Höf) and the Austrian Institute of Technology (AIT) for the technical/financial support in this research work.

References

[1] Shuai Chen. Investigation of FEM Numerical Simulation for the Process of Metal Additive Manufacturing in Macro Scale. 2019.

[2] Dan Wang, Xu Chen. Closed-loop High-fidelity Simulation Integrating Finite Element Modeling with Feedback Controls in Additive Manufacturing. 2020.

[3] Fabio Haunreiter. Numerisch basierte Schweißleistungsvorhersage für den WAM-Prozess. Master thesis. FH Technikum Wien. 2021 (non-disclosure notice).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Tailored Stiffness for the Design of Adaptive Structures with Displacement Control: A Case Study.

Axel Trautwein, Tamara Prokosch and Manfred Bischoff

Institute for Structural Mechanics
Faculty of Civil and Environmental Engineering, University of Stuttgart
Stuttgart, Germany
e-mail: {trautwein, prokosch, bischoff}@ibb.uni-stuttgart.de

Abstract: In this contribution, the role of structural stiffness in the design of adaptive structures is discussed. The focus is on displacement controlled structures. More specifically, the actuation effort should be minimized. The hypothesis is that this can be achieved by making the structure as stiff as possible against external loads and as flexible as possible against the effect of actuation. An optimization problem is formulated and an analytical case study is compared and tested with other strategies [2].

Keywords: adaptive structures, optimization, mass reduction, actuators, displacement control

1 Introduction

Adaptive structures offer the possibility of saving material and thus reduce climate-damaging emissions. By using actuators, it is possible to use smaller cross-sections than in traditional structures and still comply with displacement or stress limits [1]. If only the displacements are controlled in such adaptive structures, their stiffness is the key factor. Thus, by tailoring the stiffness, mass savings compared to traditional structures can be achieved, while, at the same time, keeping the actuation effort low. To minimize the actuation energy, it is necessary to obtain an optimal solution that fulfills the competing objectives of the structure: It should be as stiff as possible against external loads, but also as flexible as possible for the actuation effect [2].

2 Analytical case study

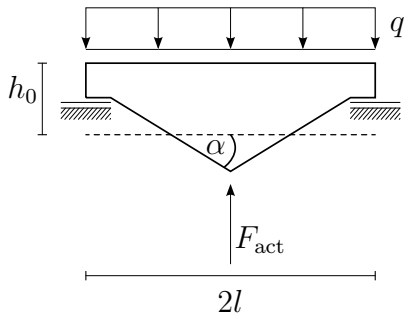


Figure 1: Tapered beam

Figure 1 shows a tapered beam with single force actuation. By the tapering constant α, the volume, respectively mass, can be distributed differently. center displacement w_l is controlled

by setting a displacement limit of $\hat{w} = 0.01$ m. As a constraint for the following optimization problems, the volume is set to $V = 1.0$ m^3. Thus, the structure cannot passively comply with the displacement limit. This very simplistic problem is chosen, because both the analysis and the underlying optimization problem are accessible to exact analytical solutions. For the hypothesis discussed at the beginning, the objective function is formulated as follows. The displacement difference in the numerator $\Delta w = w_{\text{pass}} - \hat{w}$ should be as small as possible. The displacement w_{act} produced by a unit actuation $F_{\text{act}} = 1$ in the denominator, however, should be as large as possible. In other words, the structure has to be stiff against the external load q and flexible against actuation. This can be achieved by minimizing the ratio between Δw and w_{act}. The corresponding optimization problem reads

Objective function:	$\frac{w_{\text{pass}} - \hat{w}}{w_{\text{act}}}$
Design variable:	α
Constraints:	$V = 1.0$ m^3

The optimization results in $\alpha = 0.54$. To satisfy the displacement limit, $F_{\text{act}} = 13.56$ kN is required.
Now, a holistic optimization problem is formulated. In this, F_{act} is included from the beginning and can be formalized as follows:

Objective function:	F_{act}
Design variable:	α, F_{act}
Constraints:	$w_l \leq \hat{w}$ and $V = 1.0$ m^3

This optimization approach yields exactly the same solutions for α and F_{act} as the previous one.

3 Conclusions

The initial hypothesis that the design of an adaptive load-bearing structure should be as stiff as possible with respect to the external load and as flexible as possible for the load case actuation has been validated in the given scenario. For analytical and numerical examples, this approach is identical to minimizing the actuation force. In addition (not explicitly shown above), actuation forces are lower than when the actuation is fitted to an optimized (stiffness-maximizing) passive structure. In other words, holistic approaches are superior [2].
This work was conducted in the framework of the Collaborative Research Center 1244 Adaptive Skins and Structures for the Built Environment of Tomorrow funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under project number 279064222. The authors are grateful for the generous support.

References

[1] Sobek, W., Sawodny, O., Bischoff, M., Blandini, L., Böhm, M., Haase, W., et al. (2021). *Adaptive Hüllen und Strukturen.* Bautechnik 98, 208–221. doi:10.1002/bate.202000107

[2] Trautwein, A., Prokosch, T., Senatore, G., Blandini, L. & Bischoff, M. (2023). *Analytical and Numerical Case Studies on Tailoring Stiffness for the Design of Structures with Displacement Control.* Submitted to: Frontiers in Built Environment.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Adaptation on Multi-Span Beams through Support Displacement

Lisa Schwegmann[*] and Prof. Dr. Steffen Koch[†]

[*] Department of Civil Engineering
University of Rostock
Rostock, Germany
e-mail: lisa.schwegmann@uni-rostock.de

[†] Department of Civil Engineering
University of Applied Science Wismar
Wismar, Germany
e-mail: steffen.koch@hs-wismar.de

Abstract: The construction industry causes one-third of energy consumption and emissions and is responsible for more than half of resource consumption. As a consequence of still-rising population growth and resource scarcity, engineers and architects will have to build for more people with fewer materials and emissions in the future to counteract these problems. One promising approach is adaptive load-bearing structures. Adaptivity and the integration of sensors, actuators, and materials to manipulate the construction and its characteristics (stiffness, geometry, inner forces etc.) cause material savings. The presented work concentrates on the possibilities of adaptation of multi-span beams and how these structures can be influenced especially by using deformation adaptation

Keywords: adaptivity, adaptive structures, deformation adaptation, optimization

1. Introduction

In the face of climate change and related issues like CO2 pollution, embodied energy, exhaustion of resources, and global population growth, the construction of sustainable (ultra-) lightweight structures is becoming increasingly important. There is a need for new ideas and concepts that can combat these global problems and challenges. One such idea is the use of active systems and adaptive constructions in lightweight construction, which could be significant in finding solutions to a number of these problems [1]. With adaptive systems, buildings can be created more complex, with less material and increased comfort of use. In general, adaptive structures could also provide over-dimensioning structures to safe material. With the integration of multifunctional elements (sensors, actuators, and control), the structure will be able to react to different situations and load cases. The complete structure can be controlled and manipulated actively. The adaptation is controlled with a specific algorithm. Before creating the algorithm, it´s necessary to know which properties of the system should be manipulated and what the aim of the adaption is (e.g. reduce deformations or tensions). The most important requirement for designing adaptive systems is knowledge of variable and modifiable characteristics and their influences.

2. Load Adaptation: A Case Study

In previous works different types of adaptation for multi-span beams (stiffness adaptation, cutting force adaptation, and deformation adaptation) were already investigated [2]. The results show that cutting force and deformation adaptation is significantly more efficient than influencing the stiffness. Teuffel and Sobek have already investigated the approach of deformation adaptation by support displacements [3], so this approach is also focused on here.

The optimisation objective is initially to limit or reduce the decisive moment, which means that the amount of the field and the support moment should be the same.

M Field = M Support

In the first step a support displacement is applied to a two-span beam in order to bring the two moments as close together as possible and make them equal. The considered load case refers to a 21 m HEA500 beam, which is loaded by its own weight and a single load of 50 kN. With a load position of the single load at 5 m, a support displacement of only 5 mm would have a positive effect on the moment curve and the achievement of the adaptation target (see Figure 1). The relevant moment is reduced from 121.4 kNm to 109.6 kNm.

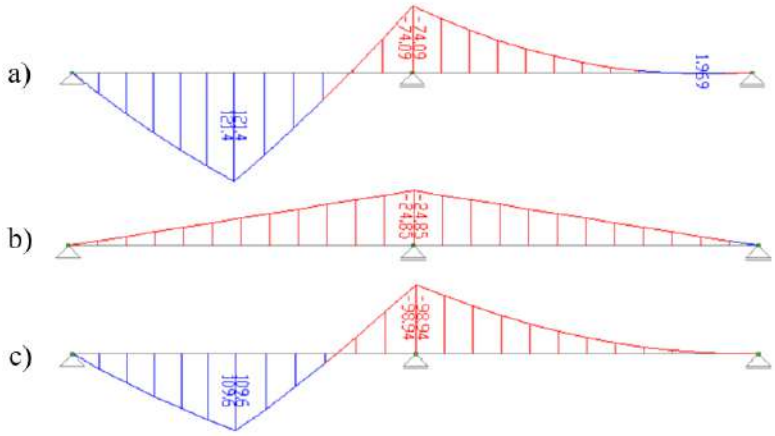


Figure 1: a) moment curve own weight and moving load; b) moment curve bearing displacement; c) superposition

3. Conclusion

The results show that a support displacement at the middle support can clearly influence the cut sizes. For more substantiated results, further load scenarios have to be investigated. For the numerical investigations (showed above) analytical solutions must be developed. Furtheremore, dynamic investigations have to be carried out, especially with regard to the application in the field of bridge construction. The dynamic investigations should concentrate on the influence of the mass inertia and the resulting correlations with regard to the positioning and actuating times of the actuators. The aim is to implement dynamic adaptation in real time, even at high velocities.

References

[1] Sobek W. et al. Adaptive Hüllen und Strukturen. Bautechnik 98, 2021

[2] Schwegmann L. Möglichkeiten der Steifigkeitsadaption bei statisch unbestimmten Trägersystemen. Master-Thesis Hochschule Wismar, 2021

[3] Sobek W. Teuffel P. Landauer A. Stuttgarter Träger. University Stuttgart, 2002

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Optimizing Flow Channels in Profile Extrusion Dies via Reinforcement Learning

Daniel Wolff[*], Clemens David Fricke[†], Marco Kemmerling[‡], and Stefanie Elgeti[†]

[*] Chair for Computational Analysis of Technical Systems (CATS)
RWTH Aachen University
Aachen, Germany
e-mail: wolff@cats.rwth-aachen.de

[†] Institute of Lightweight Design and Structural Biomechanics (ILSB)
TU Wien
Vienna, Austria
e-mail: [clemens.david.fricke|stefanie.elgeti]@tuwien.ac.at

[‡] Information Management in Mechanical Engineering (IMA)
RWTH Aachen University
Aachen, Germany
e-mail: marco.kemmerling@ima.rwth-aachen.de

Keywords: Shape Optimization, Reinforcement Learning, Profile Extrusion

Abstract

Profile extrusion is a continuous production process for manufacturing profiles from molten plastic. Especially interesting is the design of the die, through which the melt is pressed to impart the desired shape. However, due to an inhomogeneous velocity distribution at the die exit or residual stresses inside the extrudate, the final shape of the manufactured part often deviates from the desired one. By computationally optimizing the shape of the die, we aim to avoid these deviations.

We employ Reinforcement Learning (RL) for optimization, which has recently gained increasing interest in the Computational Fluid Dynamics community for tackling different challenges including shape optimization [2]. RL is based on trial-and-error interactions of an agent with an environment. For each action, the agent is rewarded and informed about the subsequent state of the environment. While not necessarily superior to classical, e.g., gradient-based or evolutionary, optimization algorithms for one single problem, RL techniques are expected to perform exceedingly well when similar optimization tasks are repeated, since the agent learns a more general strategy for generating optimal shapes instead of concentrating on just one single problem.

The feasibility of RL for optimizing profile extrusion dies has already been investigated in two previous studies [1, 3], obtaining promising results for further research. We will present a comparison of different (i.e., direct and incremental) shape optimization approaches, as well as the performance of state-of-the-art learning algorithms.

Acknowledgements This work was partially performed as part of the Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE) and received funding from the Helmholtz Association of German Research Centres. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – EXC-2023 Internet of Production – 390621612.

References

[1] Fricke, C., Wolff, D., Kemmerling, M., & Elgeti, S. (2022). Investigation of reinforcement learning for shape optimization of profile extrusion dies. 1–35. https://doi.org/10.48550/arXiv.2212.12207

[2] Garnier, P., Viquerat, J., Rabault, J., Larcher, A., Kuhnle, A., & Hachem, E. (2021). A review on deep reinforcement learning for fluid mechanics. Computers and Fluids, 225(September). https://doi.org/10.1016/j.compfluid.2021.104973

[3] Wolff, D., Fricke, C., Kemmerling, M., & Elgeti, S. (2022). Towards shape optimization of flow channels in profile extrusion dies using reinforcement learning. Proceedings in Applied Mathematics and Mechanics, 22.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Towards the Optimization of Injection Molding Processes

Blanca Ferrer Fabón* **and Marek Behr***

* Chair for Computational Analysis of Technical Systems (CATS)
RWTH Aachen University, Germany
e-mail: ferrer@cats.rwth-aachen.de

Abstract: To avoid manufacturing defects and achieve the accuracy requirements of today's industry, high-resolution and efficient numerical simulations are, in most cases, required. In the injection molding industry, the available simulations are computationally costly and often imprecise, especially during the filling stage. Designing accurate and efficient simulations is the first step towards the process' optimization.

In this work, we propose a complete model for the numerical simulation of injection molding for semi-crystalline polymers. With the purpose of preparing the simulation for solving the inverse problem, the simulation complexities and optimization potentials are identified. A local mesh refinement in areas of interest is proposed to increase the solution precision without compromising the computational time.

Keywords: Injection Molding, Optimization, Numerical Simulation, FEM, Semi-Crystalline Polymers

1 Introduction

Following the work of Karyofylli [1], in the search for efficient numerical methods for the simulation of injection molding, we work towards a more accurate solution, including the temperature problem and extending it for semi-crystalline polymers. In [2], a complete model for the injection molding representation is presented. Additionally, a study with a 2D geometry determines the relevancy of each material model. In this work, we apply the model presented in [2] with a taylored set of the relevant models and analyze the performance of the simulation in a 3D realistic geometry.

2 Governing equations and solution technique

In the proposed model, the injection molding process is described as a two-phase flow governed by the transient incompressible Navier-Stokes equations. The temperature, the crystallization for semi-crystalline polymers, and the level-set problems are also introduced to the system as transport equations coupled to the fluid equations. A detailed description of the governing equations and solution technique is available in [2]. As proposed in the latter, some model simplifications are applied in this work. Additionally, stress-induced crystallization is not considered. The simulated injected material is a semi-crystalline polypropylene, modeled as described in [2].

To discretize the governing equations, we use P1P1 finite elements with Galerkin/Least-Squares (GLS) stabilization. We use space-time elements to discretize the 3D domain. Due to the complex nature of the problem, fine discretization is a priori required; for our geometry, we use a mesh with over 1 million elements. To solve such a large problem, the typical numerical techniques, i.e., preconditioning and relaxation factors, have been applied to our simulation, adjusting the parameters for faster convergence.

3 Results

The simulated geometry is provided by the Institute of Plastics Processing (IKV) at RWTH Aachen University, and it corresponds to the one used for physical experiments at IKV. Initial and boundary conditions for the problem variables are chosen according to the experimental conditions. Solving the problem with a time-step of 0.01 seconds, the results obtained are qualitatively satisfactory. However, the computational times are still far from practical in an iterative inverse problem solver. The solution time distributions obtained after six time steps are listed in Table 1 and indicate that the incompressible Navier-Stokes (INS) solution is the costlier one, representing 87% of the total computational time. In particular, for this problem, the preconditioning step is very significant. In general, for all the problems, the system assembly is the most expensive step.

Table 1: Computational time distribution per problem and solver step, in percentages.

	INS	Lev	Temp	Cryst
Form LHS and RHS	45	43	50	37
GMRES	3	3	1	27
Preconditioner	36	14	12	0
Total	87	1	1	11

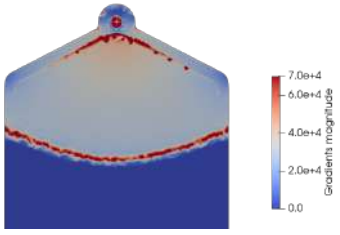


Figure 1: Pressure gradient.

Regarding the problem solution, we can detect areas with high over-/undershoots due to high solution gradients. As expected, the pressure and temperature gradients are higher near the air-polymer interface and near the domain walls. In Fig. 1, we observe high magnitudes of pressure gradients near the flow interface and near the upper sharp edge.

4 Conclusions

The Navier-Stokes problem requires noticeably more computational effort than the transport equations. Therefore, efforts should focus on improving its convergence speed. Areas where high gradients are localized are the moving interface and the walls touched by the polymer phase. This indicates that a local refinement in time and space in these areas will increase the solver's precision without compromising the computational time.

5 Acknowledgements

The authors acknowledge the support of the German Research Foundation (DFG) under program SFB 1120 "Precision Melt Engineering" - 236616214. Computations were conducted on clusters provided by RWTH Aachen University and by Jülich Aachen Research Alliance.

References

[1] V. Karyofylli, M. Behr, M. Schmitz, and C. Hopmann, Mat.-wiss. u. Werkstofftech. **48**, 1264–1269 (2017).

[2] B. Ferrer and M. Behr, Proc. Appl. Math. Mech. **19**, (2019).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Topology optimization using a Fast-Fourier-Transformation based solver with compability projection

Indre Jödicke[*], Richard Leute[*], Till Junge[†] and Lars Pastewka[*]

[*] Department of Microsystems Engineering (IMTEK)
Faculty of Engineering, University of Freiburg
Freiburg, Germany
e-mail: indre.joedicke@imtek.uni-freiburg.de

[†] Institute of Mechanical Engineering
School of Engineering, École Polytechnique Fédérale de Lausanne
Lausanne, Switzerland

Abstract: To use topology optimization for the systematic design of mechanical metamaterials it is necessary to solve the mechanical homogenization problem multiple times. In the majority of cases a Finite Element solver is used for the solution of the equilibrium, whereas Fast-Fourier-Transformation based solvers show promise to become a more efficient tool for homogenization problems. Therefore we propose to use a Fast-Fourier-Transformation based solver with compatibility projection in topology optimization. To do so, we adapt the adjoint method to calculate the gradient of topology optimization problems using a Fast-Fourier-Transformation based solver with compatibility projection. Since the proposed solver has the added advantage of being able to handle voxels with zero stiffness we show the applicability of the method on the design of some simple metamaterials, while modelling the void region with zero stiffness.

Keywords: metamaterial, topology optimization, fast fourier transform, phase field

1. Introduction

Topology optimization is a well-established method to systematically design structures and is often used in the inverse design of mechanical metamaterials. However, it remains an ongoing topic of research to reduce its high computational cost. A major contribution to these costs is the repeated solution of the mechanical homogenization problem, mostly done with a Finite Element solver. Recently, Fast-Fourier-Transformation (FFT-) based equilibrium solvers have been proposed as an efficient alternative to solve the mechanical homogenization problem in topology optimizations, e.g. [1]. We propose to use a FFT-based solver with a compatibility projection based on linear finite elements. This solver shows advantageous convergence properties while also allowing to model internal free surfaces. In addition it eliminates ringing—an oscillation problem occurring in many FFT-based solvers [2, 3]. We adapt the adjoint method—a standard method to calculate the gradients of topology optimization problems to this solver. Then we demonstrate the method by designing some simple metamaterials using zero stiffness for the void regions [4].

2. Methodology

A FFT-based solver with compatibility projection relies on a self-adjoint compatibility operator which projects every field onto its compatible part. This compatibility projection depends only on the chosen discretization and, in Fourier space, it can be calculated by a tensor product with a block-diagonal tensor. It can therefore be evaluated without high computational costs.

We use the adjoint method along with the properties of the compatibility projector to derive an efficient way of calculating the gradient of an optimization problem subjected to the discretized equilibrium equation. It consists of solving an adjoint equation which has the same structure as one Newton-iteration of the equilibrium solver. Then the sensitivity can be calculated with simple tensor products.

3. Validation

We implemented the adjoint method in the open source solver µSpectre [5]. As validation we present some relatively simple topology optimization problems: We optimize for a linear elastic metamaterial with a prescribed stiffness tensor by minimizing the difference between the actual average stress and a target average stress. The phase-field method proposed by Bourdin et al. [6] is used to make the necessary regularization of the topology optimization problem. As optimizer we chose the standard L-BFGS-B optimizer of scipy.

4. Conclusions

To conclude, we have successfully derived and implemented the adjoint method for topology optimization problems using a FFT-based solver with compatibility projection. Our examples show that the method can be used in topology optimization problems modelling void regions with zero stiffness. Thus, they open the way for more complex optimization problems.

Acknowledgements

We acknowledge funding by the Carl Zeiss Foundation (Research cluster \Interactive and Programmable Materials - IPROM").

References

[1] Cornaggia, R., & Bellis, C. (2020). Tuning effective dynamical properties of periodic media by FFT-accelerated topological optimization. Int J Numer Methods Eng 2020; 121(14): 3178-3205.

[2] Leute, R. J., Ladecký, M., Falsafi, A., Jödicke, I., Pultarová, I., Zeman, J., Junge, T. & Pastewka, L. Elimination of ringing artifacts by finite-element projection in FFT-based homogenization. J Comput Phys 2022; 453: 110931.

[3] Ladecký, M., Leute, R. J., Falsafi, A., Pultarová, I., Pastewka, L., Junge, T., & Zeman, J. Optimal FFT-accelerated Finite Element Solver for Homogenization. arXiv preprint arXiv 2022: 2203.02962.

[4] Jödicke, I., Leute, R. J., Junge, T., & Pastewka, L. Efficient topology optimization using compatibility projection in micromechanical homogenization. arXiv preprint arXiv 2021:2107.04123.

[5] https://gitlab.com/muspectre/muspectre.

[6] Bourdin, B., & Chambolle, A. (2003). Design-dependent loads in topology optimization. ESAIM: Control, Optimisation and Calculus of Variations 2003; 9:19-48.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Bead Patterns in Free-Form Shape Design Optimization

Devresse Bastian*, Geiser Armin*, Schmölz David* and Bletzinger Kai-Uwe*

* Chair of Structural Analysis
Technical University of Munich
Munich, Germany
e-mail of the atuhor: bastian.devresse@tum.de

Abstract: This work introduces a formulation of bead patterns for node-based shape optimization of the thin metal sheets manufactured by stamping. The implementation is based on the penalty formulation. The performance and final shape comparison is conducted on suitable examples.

Keywords: Shape Optimization, Vertex Morphing, Bead Patterns

1 Introduction

A great and ever-increasing number of engineering applications are formulated and solved by applying numerical methods. One of those applications is the free-form shape optimization (SO), where the node-based parameterization techniques are powerful tools for optimal shape generation [1]. A geometry parameterization called Vertex Morphing was introduced by Hojjat [2] regulating the shape updates by a filtering technique. This method has proven to enable large freedom of optimal design generation. However, due to manufacturing specifications, the patterns from traditional engineering concepts, such as beads, are often preferred by engineers.

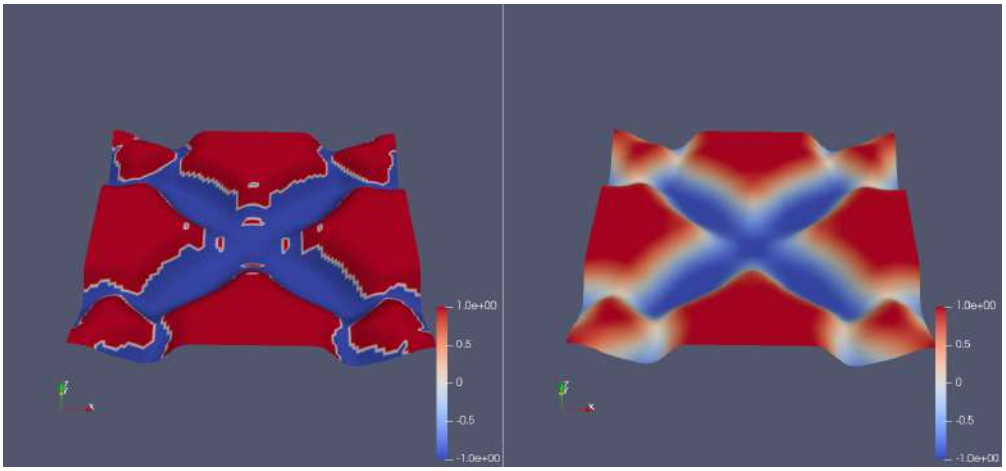


Figure 1: Discrete (left) and smooth (right) parameter values at the end of the optimization.

2 Enforcing Bead-Like Patterns

This work addresses the aforementioned challenges for the stamping manufacture process. It proposes a solution with the generation of bead-like patterns in free-form SO for thin

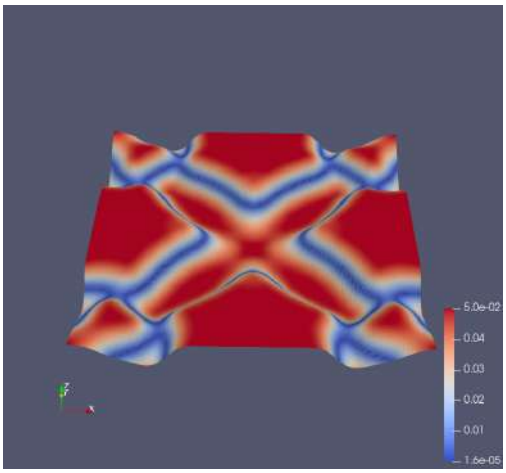


Figure 2: Absolute update colouring of the final bead pattern.

metal sheets. The presented bead optimization technique is based on the previously stated geometry parameterization technique called Vertex Morphing. Bead patterns are introduced by enforcing the creation of discrete beads in the parameterization. A penalty function forces the nodes to either bound, creating a discrete field of nodes assigned to either the upper or lower bead (figure 1 left). The Vertex Morphing technique then ensures a smooth transition by filtering the discrete field (figure 1 right).

3 Example

The proposed method is to be tested on an initially flat plate supported at the corners and loaded in the center. The optimization goal is to minimize the strain energy, thus maximizing the stiffness.

The resulting shape is depicted in figures 1 and 2. It exhibits bead patterns, thus resulting in the desired behaviour of the method.

4 Conclusions

In the example of the simple plate the method shows to effectively lead to clear bead shapes. The bead patterns can thus be created with the presented method.

References

[1] Bletzinger KU. Shape optimization. Encyclopedia of Computational Mechanics Second Edition. Wiley Online Library; 2017, p. 1-42.

[2] M. Hojjat, E. Stavropoulou, and K.-U. Bletzinger. The vertex morphing method for node- based shape optimization. Computer Methods in Applied Mechanics and Engineering 2014, 268:494–513.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Extended Vertex Morphing parameterizations for node-based shape optimization with engineering specifications

Schmölz David*, Antonau Ihar*†, Geiser Armin*, Najian Asl Reza* and Bletzinger Kai-Uwe*

* Chair of Structural Analysis
Technical University of Munich
Munich, Germany
e-mail of the author: david.schmoelz@tum.de

† Institute of Structural Analysis
Technical University of Braunschweig
Braunschweig, Germany

Abstract: The node-based shape optimization Vertex Morphing method, which originally controls the evolution of shape freely during the optimization, is adapted to meet engineering specifications. That is achieved, by changing the kernel functions of the filter procedure to satisfy geometric conditions like plane-symmetry, axis-symmetry, extrusion, curvature and others. By formulating these conditions inherently in the shape parameterization, no additional explicit constraints have to be included in the underlying optimization problem. The optimization problem can then be solved by the steepest descent method.

Keywords: Shape Optimization, Vertex Morphing, Gradient-based optimization

1 Introduction

Vertex Morphing is a successful node-based shape parameterization technique offering a rich design space introduced by Hojjat et al. [1] and Bletzinger [2] in 2014. Since then, the method has been applied to various practical shape optimization problems, directly performed from finite element models.

Engineering specifications are an important part of the optimization problem formulation and play a crucial role in the outcome of the optimization results. One can formulate the engineering specification as a geometrical constraint, usually as one constraint per node. As a result, the number of constraints is significant leading to numerical challenges. Thus, an aggregation technique might be applied and a robust constrained optimization algorithm is required to solve the optimization problem.

2 Contribution

In this work, the engineering specifications, such as plane-symmetry, axis-symmetry, extrusion, curvature and others, are formulated intrinsically in the Vertex Morphing method. The explicit filtering operation of the Vertex Morphing method generates a smooth shape x from an introduced design control field s through an integral on the surface with coordinate ξ:

$$x_i = x(\xi_i) = \int_{\xi_i - r}^{\xi_i + r} F(\xi_i, \xi, r)\ s(\xi)\ d\xi \tag{1}$$

where ξ_i is the surface coordinate of point x_i and r the radius of the filter function F. The desired geometrical properties are introduced by modifying the filter kernel function and therefore changing the shape parameterization. Hence, to solve an optimization problem with these specifications, simple unconstrained optimization methods can be used, such as the steepest descent method. Furthermore, the Vertex Morphing parameterization technique filters the shape sensitivities consistently [2], ensuring that the final solution has a good mesh quality with smooth surface and boundaries.

Numerical examples of industrial significance support the work, see e.g. Figure 1.

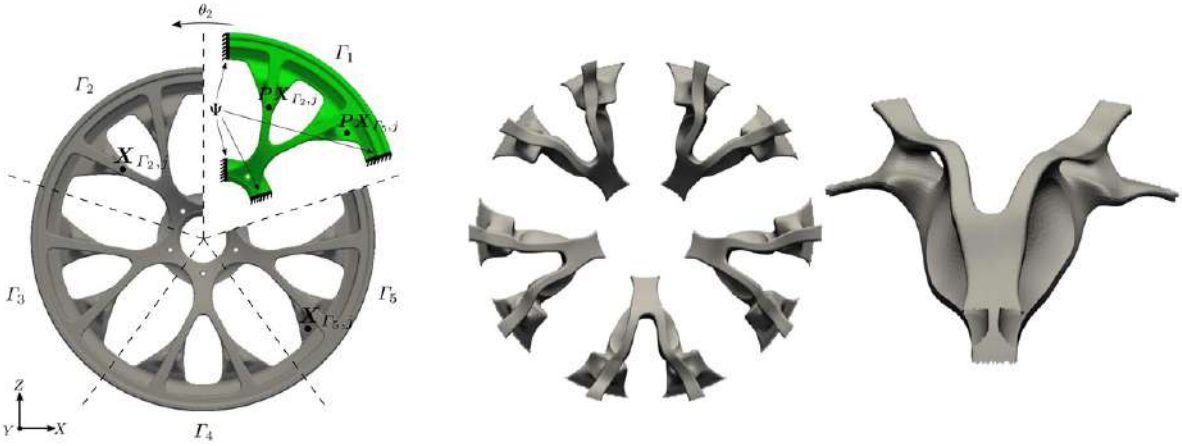


Figure 1: Axis-symmetrical Vertex Morphing: Partitioning of the rotationally symmetric wheel into 5 parts. The green part may serve as the design surface from which the whole wheel geometry can be generated. [3]

3 Conclusions

An approach to satisfy engineering specifications through an adaption of the Vertex Morphing shape parameterization has been presented. Thus, geometrical constraints don't have to be formulated in the optimization problem. Simple unconstrained optimization methods already guarantee that the design stays inside the feasible domain.

References

[1] Hojjat M, Stavropoulou E, Bletzinger KU. The Vertex Morphing method for node-based shape optimization. Computer Methods in Applied Mechanics and Engineering. 2014;268:494–513.

[2] Bletzinger KU. A consistent frame for sensitivity filtering and the vertex morphing of optimal. Structural and Multidisciplinary Optimization. 2017;49:873–895.

[3] Najian Asl R. Shape optimization and sensitivity analysis of fluids, structures, and their interaction using Vertex Morphing parametrization. Dissertation, Technical University of Munich, 2019.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Generalized approach to manufacturing constraints for node-based shape optimization using Vertex Morphing

Antonau Ihar*†, Schmölz David* and Bletzinger Kai-Uwe*

* Chair of Structural Analysis
Technical University of Munich
Munich, Germany
e-mail: ihar.antonau@tum.de

† Institute of Structural Analysis
Technical University of Braunschweig
Braunschweig, Germany

Abstract: The work presents the generalized approach to include specific manufacturing constraints in the shape optimization process. The manufacturing simulation is replaced as one particular geometrical constraint that can be easily included in the optimization workflow. The work presents several manufacturing-specific constraints and their formulations.

Keywords: Vertex Morphing, Shape Optimization, Engineering design

1 Introduction

Node-based shape optimization, such as the Vertex Morphing technique [1], has become an effective tool for design exploration, as they can be quickly set up from existing finite element models. Furthermore, each node, in general, is used as a design variable, and thus a very rich design space is obtained. However, most established manufacturing methods still suffer from limitations with respect to the geometric complexity of the final product. As a result, shapes generated by the free-form optimization process are usually not attainable.

2 Extended abstract content

This conference talk seeks to provide a general approach to imposing suitable geometric constraints for various manufacturing processes to ensure that the solution of the optimization process can be manufactured. The manufacturing methods discussed are sheet metal stamping, additive manufacturing and tube hydroforming, which are of great importance in industrial applications. For each method, appropriate geometric conditions are chosen to improve the manufacturability. In the case of additive manufacturing, these are the overhang-free property in Figure 1, which reduces the number of necessary support structures, and the stackability property, meaning how close the geometries can be packed one into another. Sheet metal stamping requires not only undercut-free designs but also smooth shapes with limited curvature in order to reduce plastic strains. And for tube hydroforming, constant cross-section perimeter and smooth shapes are beneficial.

For solving the ill-posed shape optimization problem, the node-based Vertex Morphing parameterization technique is used, filtering the shape sensitivities in a consistent manner [2].

The filtered gradients of objective and constraint functions are then applied to gradient-based optimization algorithms based on Rosens gradient projection [3].

Several examples and results of industrial significance or from engineering applications are shown.

2.1 Figures

Figure 1 shows the optimization results with AM-specific manufacturing constraint.

Figure 1: Additive Manufacturing: Overhang-free shape for an attachment structure. In transparent blue is the initial shape, and in grey the final shape .

3 Conclusions

The work presents a generalized approach to manufacturing constraints for node-based shape optimization using Vertex Morphing. Several examples and results of industrial significance or from engineering application support the proposed approach and formulations.

References

[1] Hojjat M, Stavropoulou E, Bletzinger KU. The Vertex Morphing method for node-based shape optimization. Computer Methods in Applied Mechanics and Engineering. 2014;268:494513.

[2] Bletzinger KU. A consistent frame for sensitivity filtering and the vertex morphing of optimal. Structural and Multidisciplinary Optimization. 2017;49:873895.

[3] Rosen J. The Gradient Projection Method for Nonlinear Programming, Part II, Nonlinear Constraints. Journal of the Society for Industrial and Applied Mathematics. 1961;9:514-532.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Design of an optical space instrument using thermo-mechanical topology optimization

Sanne van den Boom*, Floris van Kempen*, René Hazelebach*, Gerard Otter*, Ivan Ferrario*, Walter Zimbeck†, Benjamin Stewart†, Zachary Post†, Steven Storck† and William Swartz†

* Netherlands Institute for Applied Scientific Research (TNO)
Delft, the Netherlands
e-mail: sanne.vandenboom@tno.nl

† Johns Hopkins University Applied Physics Laboratory, Laurel, MD USA

The design and manufacturing of miniaturized optical instruments with strict performance requirements is made possible by the use of a combination of advanced design and manufacturing techniques, such as Freeform Optics, Topology Optimization (TO), coupled Structural-Thermal-Optical Performance (STOP) analysis, and Additive Manufacturing (AM). However, integrating these novel technologies into existing design workflows is not straightforward, and comes with programmatic challenges as well as technical risks.

TNO, the Dutch organization for applied scientific research, has been using topology optimization to design space instruments, enabled by additive manufacturing. As an example, the Compact Hyperspectral Air Pollution Sensor Demonstrator (CHAPS-D)[1] is an airborne imaging spectrometer demonstrator that is being developed by JHU/APL (Johns Hopkins University Applied Physics Laboratory, USA) for NASA ESTO (Earth Science Technology Office). JHU/APL designs the electronics, and manufactures, assembles, calibrates, and tests the instrument, and TNO supports this project with the instrument system architecture, optical design, the manufacturing of the mirrors, and the mechanical design using topology optimization. It is expected that the use of topology optimization will lead to better performance, because requirements on thermo-mechanical stability, gravity release, eigenfrequencies, and launch survival are considered during the optimization-enhanced design process.

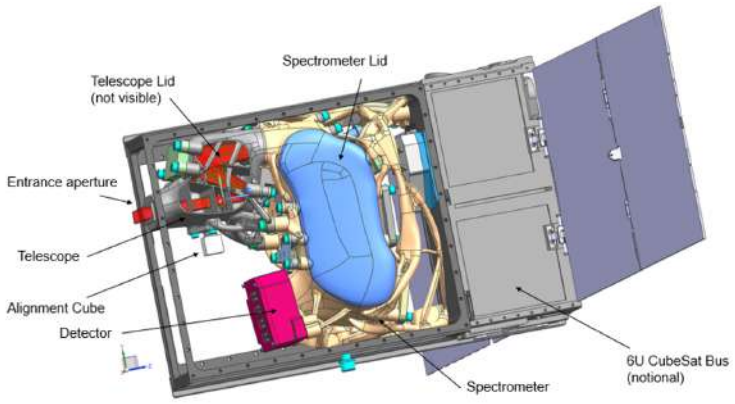


Figure 1: Design of the CHAPS-D instrument in a notional 6U CubeSat.

This presentation will focus on the approach of integrating topology optimization (TO) in existing design flows to create an optomechanical instrument, using techniques from the topology optimization literature without the use of commercial TO tools. We cover lessons learned on using topology optimization in an actual multidisciplinary design project and the additive manufacturing of the resulting designs.

References

[1] Swartz, W. H., et al. (2021), CHAPS: a sustainable approach to targeted air pollution observation from small satellites, in Proc. SPIE 11858, Sensors, Systems, and Next-Generation Satellites XXV, 1185817, doi:10.1117/12.2600175.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A discontinuity-enriched finite element method for the computational design of phononic crystals

Sanne J. van den Boom[*,†], **Alejandro M. Aragón** [*] **and Fred van Keulen**[*]

[*] Department of Precision and Microsystems Engineering
Delft University of Technology
Delft, the Netherlands

[†] Netherlands Institute for Applied Scientific Research (TNO)
Delft, the Netherlands
e-mail: sanne.vandenboom@tno.nl

Phononic crystals can be designed to have bandgaps—ranges of frequencies whose propagation through the material is prevented. They are therefore attractive for vibration isolation applications in different industries, where unwanted vibrations reduce performance. Yet, important steps are still to be made for the integration of phononic crystals into engineering practice. For instance, methods for large scale production are still in development. Furthermore, it is essential that design methods are established to enable the design of phononic crystals that meet all of the, often conflicting, requirements for practical applications. This presentation focuses on the latter challenge by proposing a computational design method for phononic crystals based on the combination of an advanced finite element method and level set-based topology optimization.

The working principle of phononic crystals is based on destructive interference of waves reflecting from the periodic arrangement of material interfaces (Bragg scattering). Consequently, it is essential that a numerical design tool accurately captures the mechanical behavior at material interfaces. Generally, in finite element analyses, this is ensured by creating a *matching* mesh: a discretization that conforms to the material interfaces. However, during computational *design*, the locations and geometry of these material interfaces change in every design iteration. One solution to this would be to create a new matching mesh for every iteration during the computational design. Nevertheless, creating new matching meshes for every design iteration is a challenging and error-prone procedure. In standard topology optimization methods this problem is commonly avoided altogether by using a density-based representation. In this approach, the discretization does not conform to the material interfaces. Instead, the interfaces are resolved by assigning a (pseudo-) density to each mesh element. As a result, these material boundaries are diffused and staircased, which is detrimental for obtaining the dynamic response of phononic crystals. The extremely fine finite element meshes required to compensate for this boundary description result in exceedingly large and expensive optimization problems.

A possible solution is to decouple the boundary description from the discretization using a level set method. Level sets have been widely used in topology optimization as an alternative design parametrization that offers more defined material boundaries. However, in most cases the level set is mapped to element densities using an Ersatz method for the analysis. Although gray values are limited to the elements that are intersected by the level set boundary, even during the optimization, the method still suffers from staircasing and diffuse

boundaries. This problem can be solved using enriched or immersed finite element methods. In these methods, standard finite element procedures are enhanced or modified to resolve material interfaces inside elements. Many such enriched and immersed methods exist, each having their own advantages and disadvantages. The work presented in this presentation focuses on the Interface-enriched Generalized Finite Element Method (IGFEM) [1], and its extensions: the Hierarchical Interface-enriched Finite Element Method (HIFEM) [2] and the Discontinuity-Enriched Finite Element Method (DE-FEM) [3]. As DE-FEM is a generalization of IGFEM/HIFEM, collectively they are also referred to as discontinuity-enriched finite element methods. An important advantage of discontinuity-enriched FEMs is the fact that *strong* enforcement of essential (Dirichlet) boundary conditions is possible on boundaries that are non-matching to the discretization mesh [4]. Because of this strong enforcement of boundary conditions, smooth reaction fields are recovered along these non-matching boundaries. It is demonstrated that this method can also be extended to the strong enforcement of Bloch-Floquet periodic boundary conditions [5], which are required for the immersed analysis of phononic crystals. This means that IGFEM is suitable for PnC design, as it can be used to modify both the phononic crystal geometry and periodicity without changing the underlying discretization, and without loss of accuracy.

Then, by creating a framework for topology optimization using IGFEM and level set functions parametrized by radial basis function, a computational design procedure is established that inherits the benefits of discontinuity-enriched methods as well as level set methods. The sensitivities required for design updates for compliance [6] as well as bandgap maximization [7] are derived analytically. Phononic crystals are optimized using the previously introduced topology optimization procedure, and we highlight the importance of accurately capturing the mechanical behavior near material interfaces for phononic crystal design. The methods introduced and developed in this work can not only be employed for the topology optimization of phononic crystals, but may also be advantageous for other optimization problems such as fluid-structure interaction or contact.

References

[1] Soghrati, S., Aragón, A.M., Duarte, A.C., Geubelle P.H. An interface-enriched generalized FEM for problems with discontinuous gradient fields, IJNME. 2012 (89) 991–1008

[2] Soghrati, S. Hierarchical interface-enriched finite element method: An automated technique for mesh-independent simulations. JCP. 2014 (275) 41 – 52

[3] Aragón, A.M., Simone, A. The Discontinuity-Enriched Finite Element Method, IJNME. 2017 (112) 1589–1613

[4] van den Boom, S.J., Zhang, J., van Keulen, F. and Aragón, A.M., A stable interfaceenriched formulation for immersed domains with strong enforcement of essential boundary conditions, IJNME. 2019 (120) 1163–1183

[5] van den Boom, S.J., van Keulen, F. and Aragón, A.M., Fully decoupling geometry from discretization in the Bloch-Floquet finite element analysis of phononic crystals, CMAME. 2021 (382) 113848

[6] van den Boom, S.J., Zhang, J., van Keulen, F. and Aragón, A.M., An Interfaced-enriched Generalized Finite Element Method for level set based topology optimization, SMO. 2021 (63) 1–20

[7] van den Boom, S.J., Abedi, R., van Keulen, F. and Aragón, A.M., A level set-based interface-enriched topology optimization for the design of phononic crystals with smooth boundaries, CMAME. 2023 (408) 115888

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Fracture scale fluid flow models for the simulation of poroelasticity

Tim Hageman [*†], **René de Borst** [†]

[*] Department of Civil and Environmental Engineering
Imperial College London
London, UK
e-mail: t.hageman@imperial.ac.uk

[†] Department of Civil and Structural Engineering
University of Sheffield
Sheffield, UK

Abstract: Fluid flows through porous materials are dominant in many applications of engineering interest. However, once cracks are introduced, often characterised by their long length but very limited opening height, computation of the fluid flows and deformations becomes costly. Here, a two-scale approach is presented which resolves the macro-scale poroelastic flow and deformation problem, coupled to a small-scale formulation for the fluid flow within the cracks. This enables the simulation of complex fluid flows, where effects such as inertia and non-Newtonian rheologies are important. The scheme is applied to a typical hydraulic fracturing case, showing its capabilities of capturing travelling pressure waves and nonlinear fluid models.

Keywords: Poroelasticity, hydro-fracture, two-scale approach, isogeometric analysis, interface elements

1 Introduction

Fluid flows in porous media are significant in a wide range of cases of engineering interest: Underground geothermal storage and resource recovery, chemical reactors, and groundwater pollution spreads, to name a few. However, these processes are often complicated by the presence of cracks and fractures. While these cracks often have very small opening heights, they can dominate the solution, making it important but usually costly to include them within computational schemes [1]. Therefore, two-scale schemes which can capture both the large-scale deformations and fluid flows, as well as the small-scale fluid flow within the cracks are important. Traditionally, these schemes have been limited to using analytic solutions for the velocity profiles within the cracks, limiting their applicability to a small range of fluids. In contrast, a scheme will be presented here that resolves the small-scale problem numerically, allowing complex phenomena such as inertia and non-Newtonian fluid rheologies to be included.

2 Model overview

To model these flows in fractured and deformable porous materials, the momentum and mass balance are used to describe the poroelastic material. Additionally, the fluid within the crack is tracked by averaging the mass balance over the total height. These three balances are

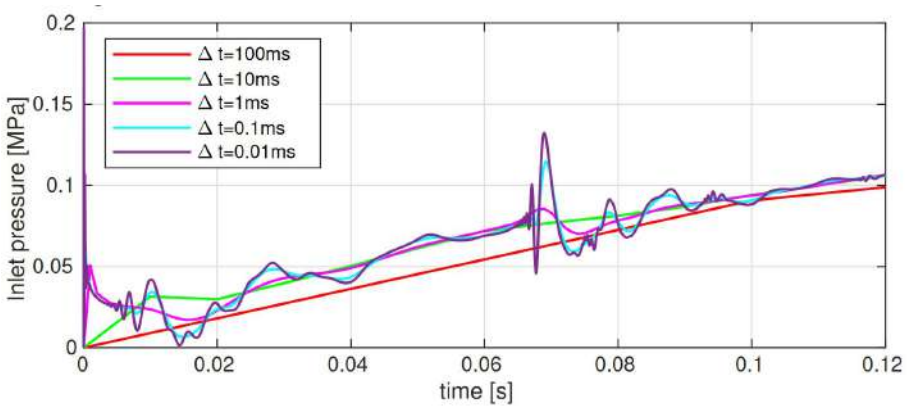


Figure 1: Results for a typical hydraulic fracturing case showing the pressure oscillations captured through the two-scale model when sufficiently small time increments are used.

given by [2]:

$$\overline{\rho}\ddot{\boldsymbol{u}}+\rho_f\dot{\boldsymbol{q}}-\boldsymbol{\nabla}\cdot(\boldsymbol{\sigma}_s-\alpha p\boldsymbol{I})=0 \qquad \frac{1}{M}\dot{p}+\alpha\boldsymbol{\nabla}\cdot\dot{\boldsymbol{u}}+\boldsymbol{\nabla}\cdot\boldsymbol{q}=0 \qquad k_i\oint(p^+ + p^- - 2p_d)+\frac{\partial q_x}{\partial x}+\dot{h}+\frac{h}{K_f}\dot{p}_d=0$$

with the degrees of freedom describing this system being the solid deformations $\boldsymbol{u}$, and the fluid pressure within the porous material and discontinuity, p and p_d respectively. The state of the system is also described through the fracture-local quantities h (crack opening height) and q_x (total fluid flux within the crack), and the constitutive equations for the solid stresses (using a linear-elastic material) and fluid fluxes (using Darcy's law):

$$\boldsymbol{\sigma}=\boldsymbol{D}\boldsymbol{\nabla}^s\boldsymbol{u} \qquad \boldsymbol{q}=-\frac{k}{\mu}\left(\boldsymbol{\nabla}p+\rho_f\left(\ddot{\boldsymbol{u}}+\frac{1}{\theta}\dot{\boldsymbol{q}}\right)\right)$$

Together, these equations above describe the full behaviour of the large-scale system. To capture the behaviour of the fluid within the crack, the small-scale is resolved as unidirectional flow via the Navier-Stokes equations, and coupled to the large-scale model by integrating the velocity over the total crack height:

$$\rho_f\dot{v}+\frac{\partial p_d}{\partial x}-\mu\frac{\partial^2 v}{\partial y^2}=0 \qquad q_x=\int_h v\,\mathrm{d}y$$

with this small-scale model being described by its velocity v. This velocity field is solved numerically within each integration point based on the large-scale displacements and pressures, and the resulting velocity is integrated and then provided to the large-scale model via the fluid flux through a scheme comparable to return-mapping schemes commonly employed for plasticity modelling. Since this scheme calculates the velocity profiles through a numerical scheme, it can also be extended to non-Newtonian fluids.

The governing equations are discretised using a finite element method, via a mesh composed of cubic and quartic Bezier extracted T-splines [3]. The fracture path is represented within this mesh as a discontinuity composed of interface elements [4], with this discontinuity being extended through a re-meshing procedure to capture the propagating crack. A consistent tangential matrix is used within the nonlinear solver to improve convergence, taking into account the contributions from the small-scale model for the fluid flow within the crack.

3 Results

The pressure at the inlet of the crack is shown in Figure 1, for a typical crack propagation case using a Newtonian fluid. At the onset of the simulation, a pressure wave travels through the crack due to the imposed inflow, with initial reflections of this wave showing 0.01 s later. This shows the ability of the described scheme to capture inertial effects within the fracture through the two-scale approach.

References

[1] Hageman, T, de Borst, R. Direct simulation vs subgrid scale modelling of fluid flow in fractured or fracturing porous media. Comp. Geosc. 2022; 26(3), 503–515.

[2] Hageman, T, de Borst, R. A refined two-scale model for Newtonian and non-Newtonian fluids in fractured poroelastic media. J. Comp. Phys. 2021; 441, 110424.

[3] Scott, MA, Borden, MJ, Verhoosel, CV, Sederberg, TW, Hughes, TJR. Isogeometric finite element data structures based on Bézier extraction of T-splines. International J. Num. Meth. Eng. 2011; 88(2), 126–156.

[4] Boone, TJ, Ingraffea, AR. A numerical procedure for simulation of hydraulically-driven fracture propagation in poroelastic media. Int. J. Num. An. Meth. Geo. 1990; 14(1), 27–47.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Fast deterministic and randomized algorithms for low-rank approximation, matrix functions, and trace estimation

Alice Cortinovis*

* Department of Mathematics
Stanford University
Stanford (CA), USA
e-mail: alicecor@stanford.edu

Abstract: This talk is based on my PhD thesis, in which we study deterministic and randomized algorithms for numerical linear algebra problems. A central theme of the thesis is that of matrices with low-rank structure: we develop and analyze algorithms for building a low-rank approximation of a matrix using some of its rows and columns, and we propose a fast algorithm for computing functions of matrices that have off-diagonal low-rank structure. Then, we consider the problem of estimating the trace of a matrix that is available implicitly, through quadratic forms. We analyze the convergence of a randomized algorithm and the connection to the approximation of the determinant of large-scale symmetric positive definite matrices.

Keywords: Numerical linear algebra, low-rank approximation, column subset selection, matrix functions, banded matrices, hierarchical matrices, Krylov methods, randomized trace estimation, Monte Carlo.

1 Introduction

Numerical linear algebra provides essential building blocks (such as the solution of linear systems or eigenvalue problems) for solving complex problems in various fields. In my thesis [1] we focused on the analysis and development of efficient algorithms with strong theoretical guarantees for numerical linear algebra problems. In particular, we considered the low-rank approximation of matrices, the computation of matrix functions, and the approximation of the trace of a matrix that is available through quadratic forms. In this talk (and in this document) a brief overview of each of these topics will be presented.

2 Low-rank approximation of matrices using rows and columns

Finding a low-rank approximation of a matrix $A \in \mathbb{R}^{m\times n}$ means finding rectangular factors $B \in \mathbb{R}^{m\times k}$ and $C \in \mathbb{R}^{n\times k}$ such that A is approximately equal to BC^T, for some target rank $k \ll \min\{n, m\}$. Almost all matrices have full rank, but in many applications, there are matrices that have a low *numerical rank*, that is, they can be well approximated by a low-rank matrix. For example, matrices with low numerical rank arise in the discretization of PDEs, in statistical machine learning, in social network analysis, and in text document analysis. Having a low-rank representation of a matrix $A \in \mathbb{R}^{m\times n}$ yields advantages in terms of storage and computational efficiency. In some applications, it is useful to consider low-rank approximations in which the factors B and C are made of, or constructed from, rows and columns of A, as this provides enhanced interpretability. In the thesis we consider cross approximation and column subset selection: we prove a priori error bounds for a

greedy algorithm for cross approximation, we develop a faster and more efficient variant of an existing algorithm for column subset selection, and we present a new deterministic polynomial-time algorithm that gives a quasi-optimal cross approximation.

3 Functions of rank-structured matrices

The second part of the thesis deals with the computation of functions of a matrix $A \in \mathbb{R}^{n\times n}$. Examples of matrix functions include the inverse of A, the square root of a symmetric positive semidefinite (SPSD) A, and the matrix exponential. More generally, one can define a matrix function $f(A)$ whenever the function f is analytic on the spectrum of A. Applications include PDEs, social network analysis, and electronic structure calculations. Here we consider matrices that have a specific low-rank structure, that is, they have off-diagonal blocks with low rank. Examples include banded matrices and hierarchically semiseparable matrices. It is well known that, in many cases, functions of such matrices retain some (approximate) low-rank structure, allowing for a memory-efficient representation of $f(A)$. In this thesis we exploit this fact, combined with the observation that if A undergoes a low-rank modification $R \in \mathbb{R}^{n\times n}$ then $f(A+R) - f(A)$ is often numerically low-rank, to develop a fast divide-and-conquer algorithm to compute functions of rank-structured matrices.

4 Randomized trace estimation

In some applications, only specific quantities associated with a matrix function are required. For example, the logarithm of the determinant of a symmetric positive definite (SPD) matrix can be expressed as the trace of the matrix logarithm of A. For a general dense matrix A, computing $f(A)$ is infeasible in a large-scale setting, and cheaper methods are needed to approximate its trace. A stochastic algorithm, the Hutchinson trace estimator, provides a way of approximating the trace of a symmetric matrix $B \in \mathbb{R}^{n\times n}$ using a few quadratic forms involving suitable random vectors. In the setting in which $B = f(A)$ is a matrix function, quadratic forms with $f(A)$ can be computed – approximately – via quadrature and Krylov subspace methods much more cheaply than the computation of the whole $f(A)$. In the third part of this thesis, we analyze the convergence properties of the Hutchinson trace estimator when it is used on a symmetric but indefinite matrix B and we apply the results to the approximation of the determinant of SPD matrices.

5 Acknowledgements

The completion of my PhD thesis would not have been possible without the help and guidance of my advisor, Prof. Daniel Kressner. I would also like to thank Stefano Massei, with whom I collaborated on some projects during my PhD. My work at EPFL was supported by the SNSF project 200020_178806.

References

[1] Cortinovis, Alice. Fast deterministic and randomized algorithms for low-rank approximation, matrix functions, and trace estimation. EPFL, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical simulation of heterogeneous materials combining Artificial Intelligence and physics-based modeling

Danoun Aymen[*,1], **Prulière Etienne** [2] **and Chemisky Yves**[1]

[1] Institute of mechanics and engineering (I2M)
Université de Bordeaux
Talence, France
e-mail: aymen.danoun1996@gmail.com, yves.chemisky@u-bordeaux.fr

[2] Institute of mechanics and engineering (I2M)
École Nationale Supérieure d'Arts et Métierso
Talence, France
e-mail: Etienne.PRULIERE@ENSAM.eu

Abstract: The new industrial constraints are nowadays pushing the limits of materials in terms of mechanical properties for advanced application fields (renewable energy, healthcare, transport). One solution to adapt the material properties to target applications is to rely on heterogeneous materials due to their excellent specific characteristics (high strength-to-weight ratio, energy absorption, mechanical resistance). However, the design of such structures can be challenging given the complexity of material mechanical responses when multiple physical mechanisms are involved at different length scales. Consequently, the evaluation of the resulting mechanical behaviors requires powerful numerical tools capable of solving highly non-linear multiscale problems. Standard methodologies including multi level finite element approaches FE^2 have been extensively developed in literature to simulate the macroscopic responses of heterogeneous structures. Nevertheless, the use of such methods still suffers from the high computational costs, therefore preventing it from being efficiently applied to multiscale structural analysis. The main objective of the present thesis is to propose a complete change of paradigm in the design and simulation of complex heterogeneous structures using hybrid models that combine physical knowledge and Artificial Neural Networks (ANN) based approaches. By adopting this strategy, we have observed a drastic downscale of the expected computational cost as well as the possibility of conducting expensive simulations on desktop computers instead of HPC clusters.

Keywords: Artificial Intelligence, Multiscale modeling, Heterogeneous materials, Homogenization, Artificial Neural Networks

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Predicting the long-term effects of mechanical overload to arterial tissue: a chemo-mechano-biological computational framework

Lauranne Maes*, Jos Vander Sloten*, and Nele Famaey*

* Department of Mechanical Engineering
KU Leuven
Leuven, Belgium
e-mail: lauranne.maes@kuleuven.be, jos.vandersloten@kuleuven.be, nele.famaey@kuleuven.be

Abstract: Mechanical overload to arterial tissue is a common occurrence after surgical intervention, causing acute damage to the tissue. On the long term, the tissue either heals or degenerates further. There is a pressing need to better understand these adaptive processes in order to steer surgical procedures towards benign long-term outcomes. A biology-informed computational model of tissue adaptation after overloading is proposed, that includes the effects of inflammatory and mechanical triggers. The model is applied to three cases-studies: damage after arterial clamping, balloon angioplasty and restenosis, and adaptation of the pulmonary interposition autograft in aortic position. The results show good correspondence with experimental observations. Moreover, the model provides improved insight in the relevant biological processes.

Keywords: Arterial tissue growth and remodeling, Constrained mixture theory, Pulmonary interposition autograft in aortic position, Restenosis, Arterial clamping

1 Introduction

Various surgical interventions, such as vascular clamping, balloon angioplasty, or stenting, induce mechanical overload to arterial tissue, often causing tissue damage. This overloading and the resulting damage trigger growth and remodeling processes in the tissue, leading to changes in mass and microstructureover time. This may signify healing of the tissue, but the remodeling processes can also cause maladaptation. It remains unclear what triggers favorable over unfavorable outcomes. Therefore, we aim to gain a better understanding of growth and remodeling processes in arterial tissue after mechanical overload through in silico modeling. Currently existing models for growth and remodeling of arterial tissue lack detailed descriptions of underlying biological processes, necessary to allow for the in silico optimization of surgical procedures.

2 Methods

2.1 Parameter identification

We use a constrained mixture formulation [1] to define the mechanical properties of arterial tissue. This enables the definition of an in vivo reference configuration of the material, rather than using the stress-free configuration as reference. This stress-free state is often unknown, and moreover different for the different tissue constituents. In order to account for these different natural states, a new iterative material parameter identification method is

developed that alternates between a prestressing algorithm and a parameter fitting procedure that optimizes the match between model data and experimental biaxial tensile test data.

2.2 Arterial tissue growth and remodeling

Growth and remodeling of arterial tissue is modeled using the classical [1] and homogenized [2] versions of the constrained mixture theory, allowing a microstructurally motivated prediction of mass turnover in the tissue. The governing equations for production and degradation of the three main load-bearing constituents in the tissue, namely elastin, collagen and smooth muscle, are defined to accurately capture biological processes. The model takes into account the effects of smooth muscle cell phenotype switching, endothelial damage, collagen production by synthetic cells, enhanced by mechanical and inflammatory triggers, and vasoactivity after administration of vasoactive agents. This model is implemented in a semi-analytical mechanical framework of a pressurized cylinder, and in finite element software to account for more realistic geometries. The model is then applied to three different case-studies: damage after arterial clamping, balloon angioplasty and restenosis, and adaptation of the pulmonary interposition autograft in aortic position.

3 Conclusions

After parameter calibration with the developed iterative fitting method, we were able to reproduce clamping experiments of mouse aortas in silico with the biology-informed growth and remodeling model. The results show good correspondence with experimental measurements of the functional integrity of smooth muscle cells. We also show that the model is able to predict both inward and outward remodeling, as observed in vivo in the context of balloon angioplasty and the resulting tissue growth and restenosis. The model also shows that collagen production in the pulmonary interposition autograft in aortic position is likely immuno-mediated rather than mechano-mediated. We were able to develop a biology-informed model of arterial tissue growth and remodeling after mechanical overload that allows for a clearer understanding of these adaptive processes. Moreover, this model is a first step towards enabling in silico medicine for the optimization of long-term surgical outcomes.

4 Acknowledgements

L. Maes was supported by the Research Foundation - Flanders through a PhD Fellowship for fundamental research (11A6519N - 11A6521N).

References

[1] Humphrey JD, Rajagopal KR. A constrained mixture model for growth and remodeling of soft tissues. Math Models Methods Appl Sci. 2002;12(03):407-430.

[2] Cyron CJ, Aydin RC, Humphrey JD. A homogenized constrained mixture (and mechanical analog) model for growth and remodeling of soft tissue. Biomech Model Mechanobiol 2016;15(6):1389-1403.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Mathematical and numerical modeling of cardiac electromechanics in ventricles with ischemic cardiomyopathy

Salvador Matteo[1]

[1] Institute for Computational and Mathematical Engineering, Stanford University, California, USA

Abstract: The cardiac function is the result of the concerted action of several physical phenomena, ranging from the cellular scale to the organ level. Among these, an important role is played by the coupling between the electrical activity of the heart and its mechanical contraction. Numerical simulations of ventricular electromechanics play nowadays a crucial role in computational cardiology and precision medicine. Indeed, it is of outmost importance to analyze and better address pathological conditions by means of anatomically accurate and biophysically detailed individualized computational models that embrace electrophysiology, mechanics and hemodynamics. In this thesis, we develop a novel electromechanical model for human ventricles affected by ischemic cardiomyopathy. We couple this 3D formulation with a 0D closed-loop circulation model by an approach that is energy preserving. Our mathematical framework keeps into account the effects of mechano-electric feedbacks, which model how mechanical stimuli are transduced into electrical signals. Moreover, it permits to classify the hemodynamic nature of tachycardia. We propose novel partitioned numerical schemes to solve this 3D-0D coupled problem, where different space-time resolutions are employed according to the specific core model. We introduce flexible and scalable intergrid transfer operators to accurately and efficiently exchange information among the Partial Differential Equations of the electromechanical model. Nested and non-nested meshes with arbitrary Finite Elements can be employed for the space discretization. Given the complexity of physics-based cardiac modeling, we also design a Machine Learning method to perform real-time electromechanical simulations. Our method allows to derive a reduced-order model (ROM), written as a system of Ordinary Differential Equations, in which the right-hand side is represented by an Artificial Neural Network (ANN), that possibly depends on a set of parameters associated with the model to be surrogated. This method is non-intrusive, as it only requires a collection of pressure and volume transients obtained from the full-order model (FOM). Once trained, the ANN-based ROM can be coupled with hemodynamic models for the blood circulation external to the heart, in the same manner as the original electromechanical model, but at a dramatically reduced computational cost. We demonstrate the effectiveness of the proposed strategy on two relevant contexts in computational cardiology. We employ the ANN-based ROM to perform global sensitivity analysis on both electromechanical and hemodynamic models. Then, we perform bayesian parameter estimation starting from noisy measurements. By replacing the FOM of cardiac electromechanics with the ANN-based ROM, we perform in a few hours of computational time all the numerical simulations, which would be unaffordable, because of their overwhelming computational cost, if carried out with the FOM.

Keywords: Cardiac electromechanics, ischemic cardiomyopathy, numerical methods, scientific machine learning, global sensitivity analysis, parameter estimation, uncertainty quantification

1 Introduction

We focus on the development, analysis and clinical validation of mathematical and numerical models in the context of human heart electromechanics. This thesis enables the study of ischemic cardiomyopathy and cardiac arrhythmias from novel and deeper perspectives, by providing valuable and patient-specific quantitative information that can be integrated in the clinical practice to improve healthcare. Given the complexity of these numerical simulations in terms of total computational times and hardware requirements, we also introduce a machine learning method that allows to derive an ANN-based surrogate model for real-time electromechanical simulations. This surrogate model can be readily employed for global sensitivity analysis or robust parameter estimation with uncertainty quantification.

2 Methods

The mathematical formulation of our electromechanical model accounts for the variability and heterogeneity in the cellular, molecular and myocardial properties driven by heart failure during short-term and long-term cardiac remodeling. Furthermore, accurate and efficient numerical schemes have been introduced to properly discretize this multiphysics and multiscale mathematical model. We design intergrid transfer operators to effectively couple Differential Equations arising from cardiac electromechanics. Primary variables can be interpolated among different (non-nested) meshes and arbitrary Finite Element spaces to account for the space resolution required by the different core models. Real-time electromechanical simulations are achieved by leveraging scientific machine learning in order to encode the pressure-volume temporal dynamics of one or multiple cardiac chambers in a very lightweight fully-connected feedforward ANN with a small amount of training samples.

3 Conclusions

We develop a comprehensive electromechanical model to address rhythm disorders, such as ventricular tachycardia and fibrillation, with an unprecedented level of detail. We validate our mathematical and numerical model by considering patient-specific geometries and we personalize it based on clinical data. Thanks to the coupling with closed-loop blood circulation, the hemodynamic impact of cardiac arrhythmias can be studied for the first time in the field of computational cardiology. Furthermore, the role of mechano-electric feedbacks on cardiovascular hemodynamics has been unraveled via high-performance computing numerical simulations. This provide a significant step forward in the understanding of severe and chaotic arrhythmias for personalized medicine. We also present an accurate and efficient surrogate model of the cardiac function that allows to encompass several applications of interest, ranging from global sensitivity analysis to robust parameter estimation with uncertainty quantification, in a few hours of computations, by using a very limited amount of computational resources. Our approach meets the requirements for clinical exploitation, as it could have important implications in the generation and calibration of cardiac digital twins, i.e. digital replicas of patient-specific human hearts, as well as treatment and surgical planning, while being compliant with Green Computing practices.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Generalised Newtonian Fluids in Cardiovascular Fluid–Structure Interaction

R. Schussnig*

* High-Performance Scientific Computing
Institute of Mathematics, University of Augsburg
Augsburg, Germany
e-mail: richard.schussnig@uni-a.de

Abstract: The modelling of the cardiovascular system and its pathologies has seen great advances in the recent past. Promising applications are patient-specific surgery planning, medical device design or parameter studies on virtual cohorts. Numerical techniques applied in this context grant access to otherwise inaccessible data, while also significantly reducing associated costs and risks. Unfortunately, long simulation turnaround times still pose a major bottleneck, restricting use in clinical practice. To reduce complexity, the rheological behaviour of blood is often neglected, which can heavily impact the solution and hence related biomarkers such as the wall shear stress. Focusing on these two aspects, this work introduces novel methods reformulatng the Navier–Stokes equations for incompressible flow of a generalised Newtonian fluid. Equivalent systems are derived, allowing for equal-order mixed formulations and time-splitting schemes, which are further extended towards fluid–structure interaction. The presented examples showcase convergence properties and applicability to patient-specific simulations of aortic dissection.

Keywords: haemodynamics, quasi-Newtonian fluid, split-step method, pressure Poisson equation, FSI

1 Introduction

Incompressible flows of viscous fluids in science, engineering and medicine are among the most challenging applications of computational fluid dynamics (CFD). So-called non-Newtonian fluids increase complexity further, introducing more involved rheological laws and related fields to the flow problem. This work addresses generalised Newtonian fluid models in finite-element-based incompressible flow and fluid–structure interaction (FSI) schemes.

2 Methods

Based on a fully consistent pressure Poisson equation (PPE), we derive (i) a stable or stabilised approach coupling velocity and pressure unknowns [1] and (ii) a split-step approach [2], decoupling velocity and pressure. Both these fundamentally different concepts are used to develop state-of-the-art CFD and FSI solvers, including linearisation, decoupling, stabilisation, adaptive timestepping, preconditioning and more practically relevant aspects.

The split-step flow solver is then coupled to an incompressible, hyperelastic 3D solid, and further combined with modelling aspects such as resistance-based outflow conditions, exterior tissue support, prestress and resolution of the tissue layers with appropriate material/fibre orientations. These models and the targeted physiological parameters severely impact standard FSI coupling schemes. We achieve robust and rapid convergence also in the medical

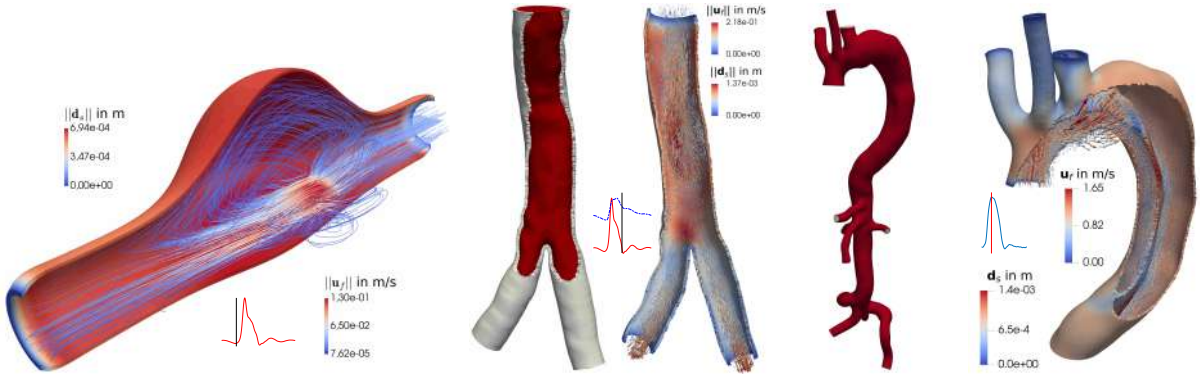


Figure 1: FSI in the cardiovascular system: flow through an abdominal aortic aneurysm [3], an iliac bifurcation [4] and an aortic dissection (flow field shown via streamlines/velocity vectors, tissue displacement color-coded in partially ommitted vessel domains).

setting with dominant added-mass effect as highlighted in Fig. 1. The partitioned coupling scheme combines Robin interface conditions and interface quasi-Newton methods, while only coupling merely the fluid pressure and structural displacement implicitly [3, 4].

3 Conclusions

The presented formulations allow for stabilised equal-order C^0-interpolation or completely decouple momentum and PPE, while rheological models are easily exchanged. Numerical examples showcase the expected convergence properties and impact of the acceleration scheme, while patient-specific simulations of aortic dissection demonstrate practical applicability.

4 Acknowledgements

The author thanks TU Graz for funding the LEAD-Project *"Mechanics, Modelling and Simulation of Aortic Dissection"*, and T.P. Fries and D.R.Q. Pacheco for the continued collaboration.

References

[1] R. Schussnig, D.R.Q. Pacheco, and T.-P. Fries. Robust stabilised finite element solvers for generalised Newtonian fluid flows. *J. Comput. Phys.*, 442:110436, 2021.

[2] D.R.Q. Pacheco, R. Schussnig, and T.-P. Fries. An efficient split-step framework for non-Newtonian incompressible flow problems with consistent pressure boundary conditions. *Comput. Methods Appl. Mech. Eng.*, 382:113888, 2021.

[3] R. Schussnig, D.R.Q. Pacheco, and T.-P. Fries. Efficient split-step schemes for fluid–structure interaction involving incompressible generalised Newtonian flows. *Comput. Struct.*, 260:106718, 2022.

[4] R. Schussnig, D.R.Q. Pacheco, M. Kaltenbacher, and T.-P. Fries. Semi-implicit fluid–structure interaction in biomedical applications. *Comput. Methods Appl. Mech. Eng.*, 400: 115489, 2022.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Existence Results for Ferromagnetic Elastomers

Marco Bresciani*, Manuel Friedrich* and Carlos Mora-Corral†

* Department of Mathematics
Faculty of Sciences, Friedrich-Alexander-Universität Erlangen-Nürnberg
Erlangen, Germany
e-mail: marco.bresciani@fau.de; manuel.friedrich@fau.de

† Department of Mathematics
Faculty of Sciences, Universidad Autónoma de Madrid
Madrid, Spain
e-mail: carlos.mora@uam.es

Abstract: We study a variational model for ferromagnetic elastomers at large strains. The characteristic feature of the model consists in its mixed Eulerian-Lagrangian formulation: while deformations are classically defined on the reference configuration, magnetization fields are set on the deformed configuration in the actual space. We prove the existence of equilibrium configurations given by minimizers of the magnetoelastic energy. We start by focusing on purely elastic materials. Subsequently, we include material failure into the picture by examining soft and brittle materials that may undergo cavitation and fracture, respectively.

Keywords: Magnetoelasticity, Calculus of Variations, Direct Method, Free-discontinuity Problems

1 Introduction

Magnetoelastic materials are characterized by their tendency to experience mechanical deformations in response to external magnetic fields. This peculiar behaviour is termed magnetostriction and constitutes the foundation of the technology behind many devices such as sensors and actuators.

A first phenomenological theory of magnetoelasticity has been proposed by Brown in the form of a **variational principle** [5]. Let $\Omega \subset \mathbb{R}^3$ represent the reference configuration of a magnetoelastic body subject to deformations $\boldsymbol{y}\colon \Omega \to \mathbb{R}^3$ and magnetizations $\boldsymbol{m}\colon \boldsymbol{y}(\Omega) \to \mathbb{R}^3$. Neglecting thermal effects, magnetizations must comply with the **saturation constraint**

$$|\boldsymbol{m} \circ \boldsymbol{y}| \det D\boldsymbol{y} = 1 \text{ in } \Omega. \tag{1}$$

Equilibrium configurations are given by minimizers of the magnetoelastic energy functional

$$(\boldsymbol{y}, \boldsymbol{m}) \mapsto \int_\Omega W(D\boldsymbol{y}, \boldsymbol{m} \circ \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} + \int_{\boldsymbol{y}(\Omega)} |D\boldsymbol{m}|^2 \, \mathrm{d}\boldsymbol{\xi} + \frac{1}{2} \int_{\mathbb{R}^3} |Du_{\boldsymbol{m}}|^2 \, \mathrm{d}\boldsymbol{\xi}, \tag{2}$$

where $\boldsymbol{x}$ and $\boldsymbol{\xi}$ denote Lagrangian and Eulerian variables, respectively. The three terms correspond to the elastic, exchange and magnetostatic energy. The stray-field potential $u_{\boldsymbol{m}}\colon \mathbb{R}^3 \to \mathbb{R}$ is defined as a solution of the **Maxwell equation**

$$\operatorname{div}\Big(-Du_{\boldsymbol{m}} + \chi_{\boldsymbol{y}(\Omega)}\boldsymbol{m}\Big) = 0 \text{ in } \mathbb{R}^3, \tag{3}$$

where $\chi_{\boldsymbol{y}(\Omega)}\boldsymbol{m}$ simply denotes the extension of $\boldsymbol{m}$ by zero outside of $\boldsymbol{y}(\Omega)$. Applied loads given by mechanical forces and external magnetic fields can also be included.

The existence of minimizers of the functional (2) subject to the constraints in (1) and (3) is generally proved by employing the **direct method** of the calculus of variations. The implementation of this approach to our problem is very delicate, since one has to deal with the deformed configuration $\boldsymbol{y}(\Omega)$, which is unknown, and with the composition $\boldsymbol{m} \circ \boldsymbol{y}$. Still, this approach has been successfully applied and the existence of minimizers has been established by progressively relaxing the coercivity assumptions on the density W [2, 3, 4, 8, 10]. These assumptions implicitly set the regularity of deformations which, in turn, allows for a suitable interpretation of the deformed set and the specification of the regularity of magnetizations. We point out that in the above mentioned works, apart from [10], the constraint in (1) is replaced by $|\boldsymbol{m}| = 1$ in $\boldsymbol{y}(\Omega)$.

2 Main results

In the present contribution, we prove the existence of solutions for the minimization problem determined by (1)–(3).

First, we examine **purely elastic materials**. In that case, the class of admissible deformations is the same considered in [3]; these maps belong to the space $W^{1,p}(\Omega;\mathbb{R}^3)$ for some fixed $p > 2$, but cannot create cavities. Magnetizations are modeled as maps $\boldsymbol{m} \in W^{1,2}(\mathrm{im}_{\mathrm{T}}(\boldsymbol{y},\Omega);\mathbb{R}^3)$ satisfying (1). Here, $\mathrm{im}_{\mathrm{T}}(\boldsymbol{y},\Omega)$ denotes the topological image of $\boldsymbol{y}$ which, in this setting, coincides with the geometric image $\mathrm{im}_{\mathrm{G}}(\boldsymbol{y},\Omega)$ up to negligible sets [3].

Subsequently, we focus on **soft materials**. The functional setting is the same above, although deformations are now allowed to create cavities [6]. Accordingly, magnetizations are assumed to vanish within the cavity volumes. In order to recover the lower semicontinuity of the elastic energy, as in [9], we penalized the creation of new surface by adding the perimeter of the geometric image to the functional in (2).

Eventually, we investigate **brittle materials** possibly experiencing fracture. In this setting, deformations belong to the space $SBV(\Omega;\mathbb{R}^3)$ of special maps of bounded variation [1]. As the topological degree is not available for such maps, we solely resort on the notion of geometric image. Magnetizations are defined as maps $\boldsymbol{m}\colon \mathrm{im}_{\mathrm{G}}(\boldsymbol{y},\Omega) \to \mathbb{R}^3$ such that $\chi_{\mathrm{im}_{\mathrm{G}}(\boldsymbol{y},\Omega)}\boldsymbol{m} \in SBV^2(\mathbb{R}^3;\mathbb{R}^3)$ and (1). In addition to the perimeter of the geometric image, the energy functional controls the area of the jump set $J_{\boldsymbol{y}}$ of $\boldsymbol{y}$. In turns out that jumps of $\boldsymbol{m}$ inside the geometric image cannot be avoided; therefore, we penalize also the area of $J_{\boldsymbol{m}}$.

References

[1] Ambrosio L, Fusco N, Pallara D. Functions of Bounded Variation and Free Discontinuity Problems. New York: Oxford University Press; 2000.

[2] Barchiesi M, DeSimone A. Frank energy for nematic elastomers: a nonlinear model. ESAIM Control Optim Calc Var 2015; 21(2):372-377.

[3] Barchiesi M, Henao D, Mora-Corral C. Local invertibility in Sobolev spaces with ap-

plications to nematic elastomers and magnetoelasticity. Arch Ration Mech Anal 2017; 224(2):743-816.

[4] Bresciani M, Davoli E, Kružík M. Existence results in large-strain magnetoelasticity. Ann Inst Henri Poincaré Anal Non Linéaire 2022 (Online first).

[5] Brown Jr W F. Magnetoelastic Interactions. Berlin: Springer; 1966.

[6] Henao D, Mora-Corral C. Lusin's condition and the distributional determinant for deformations with finite energy. Adv Calc Var 2021; 5:355-409.

[7] Henao D, Stroffolini B. Orlicz-Sobolev nematic elastomers. Nonlinear Anal 2020; 194: 111513.

[8] Kružík M, Stefanelli U, Zeman J. Existence results for incompressible magnetoelasticity. Discrete Contin Dyn Syst 2015; 35(6):2615-2623.

[9] Müller S, Spector S J. An Existence Theory for Nonlinear Elasticity that Allows from Cavitation. Arch Ration Mech Anal 1995; 131(1):1-66.

[10] Rybka P, Luskin M. Existence of energy minimizers for magnetostrictive materials. SIAM J Math Anal 2005; 36(6):2004-2019.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Control and Optimization of Physical Systems: Quantum Dynamics and Magnetic Confinement in Stellarators

Rémi ROBIN*

*Laboratoire de Physique de l'École Normale Supérieure, Mines Paris, Inria, CNRS, ENS-PSL, Sorbonne Université, PSL Research University,
Paris, France
e-mail: remi.robin@inria.fr

Abstract: This PhD thesis deals with the optimization and control of several physical systems. It is divided into three parts.

The first part is devoted to stellarators. This type of nuclear fusion reactor poses many challenges related to optimization. We focus on an inverse problem well known to physicists, modeling the optimal design of superconducting coils generating a given magnetic field. We conduct both a theoretical and a numerical study of an extension of this problem, involving shape optimization. Then, we develop a new method to prove the existence of optimal shapes in the case of hypersurface optimization problems. Finally, we study and optimize the Laplace forces acting on a current surface density.

The second part of this thesis deals with the control of finite dimensional quantum systems. We rigorously study the combination of the rotating wave approximation with the adiabatic approximation. First, we obtain the robustness of a population transfer method on qubits. The latter then allows to extend results of Li and Khaneja on the ensemble control of qubits by restricting to the use of a single control. We also present a second contribution, devoted to the analysis of a chattering phenomenon for an optimal control problem of a quantum system.

Finally, the third part is dedicated to the proof of a small-time global null controllability result for generalized Burgers' equations using a boundary layer.

Keywords: Optimal control, quantum control, ensemble controlability, Qubit, Shape Optimization, Plasma physics, Stellarator, Burgers equation, boundary layer

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Mixed-dimensional finite element formulations for beam-to-solid interaction

Ivo Steinbrecher*

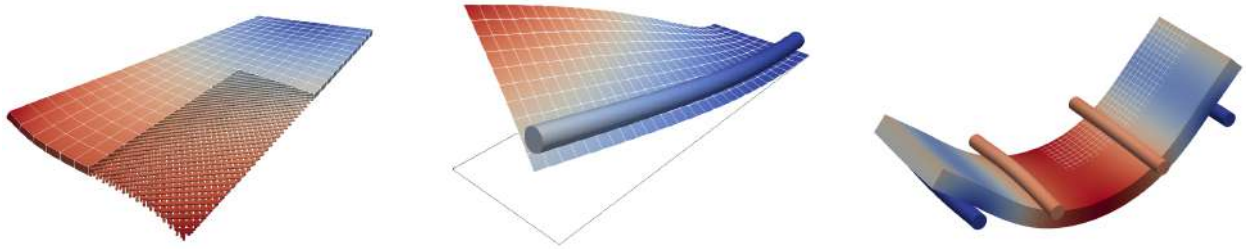
* Institute for Mathematics and Computer-Based Simulation (IMCS)
University of the Bundeswehr Munich, Neubiberg, Germany
e-mail: ivo.steinbrecher@unibw.de

Abstract: The main goal of the presented thesis is the development of finite element formulations to model the interaction between slender continua based on reduced dimensional beam theory and classical three dimensional continua (solids), i.e., a beam-to-solid interaction problem. The developed framework allows for a very flexible modeling and meshing process of the combined beam-to-solid problem and results in a drastically reduced computational effort compared to fully resolved models. Mortar-type methods are employed to discretize the coupling constraints. The approach is verified through theoretical considerations and numerical examples. The presented framework is an efficient, robust, and accurate tool for beam-to-solid interaction problems with potential applications in various fields of science and engineering.

Keywords: Mixed-dimensional interaction, Finite element method, Nonlinear beam theory, Mortar methods, Beam-to-solid coupling, Beam-to-solid contact, Fiber-reinforced materials

The interaction between slender fiber- or rod-like components, where one spatial dimension is much larger than the other two, with three-dimensional structures (solids) is an essential mechanism of mechanical systems in numerous fields of science, engineering and bio-mechanics. Examples include reinforced concrete, supported concrete slabs and fiber-reinforced composite materials. Applications can also be found in medicine, where stent grafts are a commonly used device for endovascular aneurysm repair, and in many biological systems such as arterial wall tissue with collagen fibers. The different types of dimensionality of the interacting bodies, i.e., slender, almost one-dimensional fibers and general three-dimensional solids, pose a significant challenge for typical numerical simulation methods. Classical modeling techniques usually require a compromise between a detailed description of the one-dimensional structures and overall model complexity.

The main focus of the presented thesis [1] is the development of novel computational approaches to simulate the interaction between fiber-like structures and three-dimensional solids. The key idea therein is to explicitly model the slender components as one-dimensional Cosserat continua based on the geometrically exact beam theory, which allows for an accurate and efficient description of the slender fibers (beams). Since the dimensions of the coupled differential equations are not equal, the resulting combined interaction problem is a mixed-dimensional beam-to-solid interaction problem. Not only the governing equations of the beam but also the developed interaction schemes are exclusively formulated along the one-dimensional beam centerline. From a mechanical point of view, the resulting mixed-dimensional interaction of nonlinear geometrically exact beam finite elements with classical continuum finite elements introduces a singular solution, similar to the problem of a concentrated line load acting on a three-dimensional continuum. As one of the main contributions of the thesis, theoretical considerations and numerical examples verify that this singularity does not affect the usability of the proposed methods within the envisioned application range.



(a) (b) (c)

Figure 1: Illustration of various beam-to-solid application scenarios – fiber-reinforced composite plate (a), supported plate (b) and four-point bending test (c).

Based on the considered applications, two different types of interacting geometry pairs can be identified: line-to-volume, i.e., beams embedded in solid volumes, and line-to-surface, i.e., beams tied or in contact with the surface of a solid volume. Application examples are illustrated in Figure 1. Within the presented work, coupling (i.e., tying) of the beam centerline position to the underlying solid in line-to-volume problems is investigated first. As a next step, also the rotations of the Cosserat continua are coupled to the solid volume. This requires the construction of a suitable rotation (i.e., triad) field inside the solid (Boltzmann) continuum. For both, positional and rotational coupling, mortar-type methods, inspired by classical mortar methods from domain decomposition or surface-to-surface interface problems, are employed to discretize the coupling constraints. A penalty regularization is performed to eliminate the Lagrange multipliers from the global system of equations, which results in a robust coupling scheme. This is verified by several numerical examples, in which consistent spatial convergence behavior can be achieved and potential locking effects can be avoided. In a next step, the previously developed algorithms for line-to-volume coupling to line-to-surface coupling. This introduces the additional complexity of having to account for the surface normal vector in the positional coupling constraints. It is demonstrated that only a consistent handling of the surface normal vector leads to physically accurate results and guarantees fundamental mechanical properties such as conservation of angular momentum. Finally, a beam-to-solid surface contact scheme that allows for the modeling of unilateral contact between one-dimensional beams and two-dimensional solid surfaces is presented.

The previously mentioned building blocks constitute a novel mixed-dimensional beam-to-solid interaction framework, which is verified by theoretical discussions and numerical examples throughout the thesis. Possible extensions are outlined and propose numerical and algorithmic improvements as well as the treatment of other physical effects such as delamination between embedded beams and the surrounding volume. However, already in the current state, the presented framework is an efficient, robust, and accurate tool for beam-to-solid interaction problems and can become a valuable tool in science and engineering.

References

[1] Steinbrecher, I.: Mixed-dimensional finite element formulations for beam-to-solid interaction. Ph.D. thesis, University of the Bundeswehr Munich (2022)

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Dynamic response of arching masonry walls subjected to blast loads

Idan E. Edri

National Building Research Institute, Technion - Israel Institute of Technology, Haifa, Israel
e-mail: edri@technion.ac.il

Abstract: This research studies the blast response of arching masonry walls through combined experimental and theoretical methodologies. The experimental part includes monotonic and cyclic tests on small-size masonry specimens and a laboratory blast test on a full-size wall using a blast simulator. The theoretical part includes the development of four analytical models for the dynamic analysis applying different structural resolution levels. The first model assumes a single-degree-of-freedom response, while the other three account for the multi-degree-of-freedom nature of the response. The physical modeling assumptions in each model are discussed, and their effect on the assessment of the wall response is highlighted. The static and dynamic tests are used as benchmarks for validation of the theoretical models, and physical features of the response are discussed through a series of numerical studies. The combined experimental and theoretical effort provides insight into the complex behavior of such walls, sets quantitative tools for its analysis, and demonstrates the unique aspects of the blast response of arching masonry walls.

Keywords: Masonry wall, Arching, Blast, Dynamic response, Experiment

1. Introduction

Explosion events throughout the world have drawn attention to the vulnerability of buildings, in general, and particularly of the unreinforced masonry (URM) walls that cover a major part of the building facades. The dynamic response of such walls to the blast action is a complex structural mechanism that combines a spectrum of nonlinear and dynamic effects. This research aims at enhancing the understanding of the one-way dynamic response of arching URM walls subjected to blast loads through combined experimental and theoretical methodologies.

2. Theoretical and experimental investigation

The main part of the research is theoretical, and it includes the development of a series of four analytical models differing in the level of structural resolution. The first model (see the ARCH model in Edri and Yankelevsky [1]) assumes a simplified SDOF response. The model is based on the analytical model developed in Edri and Yankelevsky [2] for calculating the static force-displacement relation. Despite its capabilities, the ARCH model assumes a three-hinged-arch mechanism and the response is limited accordingly. To release this geometrical constraint and allow the development of more complex modes of dynamic deformation, a more sophisticated model was needed. This motivated the development of the SIM model in Edri et al. [3,4] which takes a step forward in terms of the structural resolution level by characterizing the response by means of a multi-degree-of-freedom (MDOF) modeling. The masonry units are modeled as rigid bodies, whereas the mortar joints are represented by arrays of springs with nonlinear kinematic and constitutive relations. To take a deeper look into the stress field within each mortar joint, a richer physical modeling technique was proposed in Edri et al. [5] that develops the dynamic BIM model. The physical modeling in this case also assumes rigid blocks, but now represents the mortar joints by nonlinear beam members. In the above three models, the blocks are assumed rigid. In Edri et al. [6], the level of the structural resolution is further refined by developing a continuous beam-type model (CBM model) where the flexibility of the masonry

units and the mortar joints are considered. In that sense, the model augments the above models and generalizes the structural modeling of masonry walls.
The experimental part includes monotonic and cyclic static tests on small-size masonry specimens (see Edri et al. [7]), and laboratory dynamic blast tests on a full-size wall using a blast simulator (see Edri et al. [8]). New experimental data is provided for the global and local measures of the response, quantifying the arching mechanism from macro and micro perspectives. These tests supported the theoretical work and provided additional experimental data for the examination and evaluation of the developed models.

3. Conclusions

The study has looked into the dynamic characteristics of the wall behavior through numerical investigation of the complex cracking evolution, the dynamic arching mechanism, and the features of its inelastic response and rocking. Overall, the static and dynamic experiments incorporated in the context of the present research have provided new data for the examination and evaluation of the developed models, quantified the static and dynamic response, and illuminated the arching mechanism through macro and micro perspectives. The findings of the analyses, the experimental work, and the numerical studies have indicated that the blast response of arching URM walls is characterized by unique nonlinear phenomena that affect the behavior and the analysis of such walls. The spectrum of analytical models, with different levels of resolution of the structural modeling, has set theoretical platforms for the static and dynamic analysis of the arching wall, clarified its response, and provided inclusive insight into its nonlinear behavior. It has also proposed a variety of modeling capabilities that eventually provide a possible trade-off between computation time, resolution, and accuracy.

Acknowledgements

The research was carried out under the supervision of Prof. Oded Rabinovitch and Prof. Emeritus David Yankelevsky in the Faculty of Civil and Environmental Engineering, Technion-Israel Institute of Technology.

References

[1] Edri IE, Yankelevsky DZ. Analytical model for the dynamic response of blast-loaded arching masonry walls. Eng Struct 2018;176. doi:10.1016/j.engstruct.2018.08.053.

[2] Edri IE, Yankelevsky DZ. An analytical model for the out-of-plane response of URM walls to different lateral static loads. Eng Struct 2017;136. doi:10.1016/j.engstruct.2017.01.001.

[3] Edri IE, Yankelevsky DZ, Rabinovitch O. Out-of-plane response of arching masonry walls to static loads. Eng Struct 2019;201. doi:10.1016/j.engstruct.2019.109801.

[4] Edri IE, Yankelevsky DZ, Rabinovitch O. Blast response of one-way arching masonry walls. Int J Impact Eng 2020;141:103568. doi:10.1016/j.ijimpeng.2020.103568.

[5] Edri IE, Yankelevsky DZ, Rabinovitch O. Nonlinear Rigid–Flexible Multibody Modeling of Arching Masonry Walls Subjected to Blast Loading. J Eng Mech 2021;147:04021002. doi:10.1061/(ASCE)EM.1943-7889.0001894.

[6] Edri IE, Yankelevsky DZ, Rabinovitch O. Continuous beam-type model for the static analysis of arching masonry walls. Eur J Mech - A/Solids 2021:104387. doi:10.1016/J.EUROMECHSOL.2021.104387.

[7] Edri IE, Yankelevsky DZ, Rabinovitch O. Experimental study on one-way arching masonry specimens under monotonic and cyclic loads. Structures 2022;37:1142–56. doi:10.1016/J.ISTRUC.2022.01.046.

[8] Edri IE, Yankelevsky DZ, Remennikov AM, Rabinovitch O. Combined experimental and theoretical study on the blast response of arching masonry walls. Int J Impact Eng 2023:104495. doi:10.1016/J.IJIMPENG.2023.104495.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

The Direct Parametrisation Method for Invariant Manifolds: Developments and Application to Large Dimensional Finite Element Models of MEMS Structures

Opreni Andrea*

* Department of Civil and Environmental Engineering
Politecnico di Milano
Milan, Italy
e-mail: andrea.opreni@polimi.it

Abstract: In the present work we propose a comprehensive technique to derive reduced models of nonlinear dynamical systems stemming finite element discretisation of continuum mechanics problems. The approach is based on a reformulation of the parametrisation method for invariant manifolds initially developed by Cabré, Fontich, and de la Llave and we exploit the introduction of nonlinear lifting operators from the physical space to normal coordinates defined over an invariant span of the phase space. The method is applied to the computation of bifurcation diagrams for periodic orbits of resonating micro electro mechanical systems and results are compared with solutions computed from full order simulations. The accuracy and the efficiency of the proposed reduction procedure make the presented approach a milestone in the field of nonlinear vibrations.

Keywords: Model Order Reduction, Nonlinear Dynamics, Invariant Manifold, Periodic Orbits, Vibrations

1 The direct parametrisation method for invariant manifolds

The parametrisation method for invariant manifolds (PIM) [1] sets the mathematical framework for deriving efficient reduced models of dynamical systems by parametrising the system motion along invariant spans of the phase space. However, the original formulation of the method features two main limitations associated to its application on high dimensional models, namely the necessity to rewrite the dynamical system in modal coordinates, hence requiring the knowledge of the full eigenspectrum of the system [1], and the necessity to compute nonlinear tensors for the original finite element model [2]. In the present work we propose a reformulation of the parametrisation method for invariant manifolds in direct form (DPIM) by introducing nonlinear lifting operators that map coordinates defined over an invariant set to the physical coordinates of the finite element model [3, 4, 5]. Furthermore, by operating the coordinate change on the approximated fields, we avoid the explicit computation of the nonlinearity tensors, hence avoiding memory constraints reported by similar developments [2].
A major field of application of the presented methodology is that of nonlinear vibrations and the industrial field of interest is the semiconductor industry since computation of bifurcation diagrams for periodic orbits is an essential step to optimize the behaviour at resonance of microsystems used in most electronic devices such as gyroscopes, resonant accelerometers, and micromirrors. This class of dynamical systems is described by the following equation:

$$\mathbf{M}\ddot{\mathbf{U}} + \mathbf{C}\dot{\mathbf{U}} + \mathbf{K}\mathbf{U} + \boldsymbol{G}(\mathbf{U},\mathbf{U}) + \boldsymbol{H}(\mathbf{U},\mathbf{U},\mathbf{U}) = \mathbf{F}, \tag{1}$$

with $\mathbf{M}$ mass matrix, $\mathbf{C}$ damping matrix, $\mathbf{K}$ stiffness matrix, $\boldsymbol{G}$ quadratic nonlinear operator, $\boldsymbol{H}$ cubic nonlinear operator, $\mathbf{F}$ external forcing, and $\mathbf{U}$ displacement field. The system is non-conservative and non-autonomous. Dimensionality reduction is performed by introducing a time-dependent coordinate change between nodal displacements $\mathbf{U}$, velocity $\mathbf{V} = \dot{\mathbf{U}}$ and the normal coordinates, i.e. the coordinates defined along the invariant set over which we parametrise the system motion following the procedure detailed in [5].
As an example, the method is here applied for predicting the nonlinear dynamic response of the MEMS arch resonator reported in Fig. 1(a). The device features a 1:2 internal resonance relation between the eigenfunctions reported in Fig. 1(b) and Fig. 1(c). The reduced model is performed by parametrising the system motion along the four-dimensional invariant set associated to the two eigenmodes. In Fig. 1(d) we report the bifurcation diagram computed by imposing an harmonic forcing with frequency Ω on the device and we compare the results with full order simulations. The match is perfect and the total computation time for the bifurcation diagram was lower than three minutes with the DPIM, a performance that sets a new standard in the field of nonlinear vibrations.

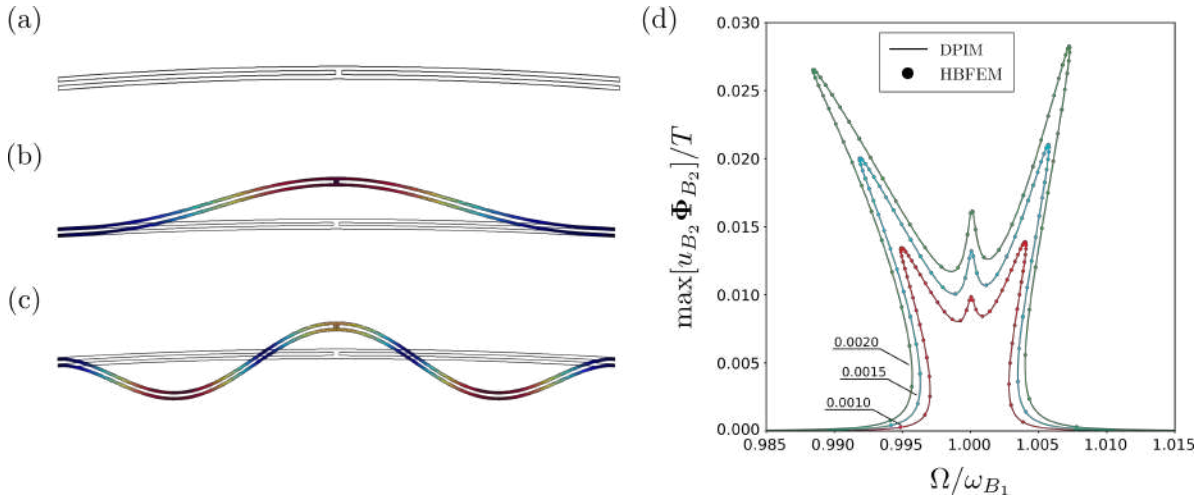


Figure 1: (a) example MEMS structure. (b-c) coupled modes in 1:2 internal resonance. (d) comparison between proposed method (DPIM) and full order harmonic balance finite element (HBFEM) solutions. The frequency is normalised by the eigenfrequency of the first mode ω_{B_1}. Along the y-axis we report the modal amplitude for the mode in (c) u_{B_2} scaled by its mode shape $\boldsymbol{\Phi}_{B_2}$ and normalised by the arch thickness T. Diagrams are computed for three forcing $\mathbf{F}$ values, whose intensity is reported as tags in the picture.

References

[1] X. Cabré, E. Fontich, R. de la Llave, J. Differ. Equ., 218(2), 444-515, (2005).

[2] S. Jain, G. Haller, Nonlinear Dyn., 107, 1417–1450 (2022).

[3] A. Opreni, A. Vizzaccaro, A. Frangi, C. Touzé, Nonlinear Dyn., 105, 1237–1272 (2021).

[4] A. Vizzaccaro, A. Opreni, L. Salles, A. Frangi, C. Touzé, Nonlinear Dyn., 110, 525–571 (2022).

[5] A. Opreni, A. Vizzaccaro, C. Touzé, A. Frangi, Nonlinear Dyn., 111, 5401–5447 (2023).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Efficient algorithms for three-dimensional computational mesh generations and air pollution simulations based on hypergraph grammars

Krzysztof Podsiadło*

* Institute of Computer Science
Faculty of Computer Science, Engineering and Communication
AGH University of Science and Technology in Kraków
Kraków, Poland
e-mail: krzysztof.podsiadlo@gmail.com

Abstract: Computer simulations solving non-stationary problems such as the propagation of air pollutants using the finite element method are currently considered a hot scientific topic. This is because there is a need to reduce the computational cost of classical algorithms and the need to control the correctness of the computational process automatically. Expressing the computational process through the production of hypergraph grammar can solve both problems. The thesis aims to design, implement, and test a new class of graph-grammar-based algorithms for the generation of computational meshes and air pollution simulations. They employ the finite element method solver based on the advection-reaction-diffusion formulation and use the graph representation of the computational mesh adaptively built with the triangular finite elements, constructed basing on the terrain topographic data. In particular, the computational mesh generation process was expressed by the graph-grammar productions, the generation of three-dimensional tetrahedral meshes filling the atmosphere on top of the terrain mesh, and the graph-grammar productions expressing the matrix free iterative solver algorithm. The graph-grammar productions are executed in parallel over mesh elements. They multiply the element matrices by the right-hand side vector and assemble to global right-hand side vector. The expression of the mesh generation and solver algorithm by graph-grammar productions allows for efficient parallel simulations of the pollution propagation process.

Keywords: Finite Element Method, Graph grammars, Air pollution simulations, Matrix free solver

1 Introduction

Computer simulations solving non-stationary problems such as the propagation of air pollutants using the finite element method are currently considered a hot scientific topic. The reason of it is a need to reduce the computational cost of classical algorithms and the need to control the correctness of the computational process automatically. The dissertation aims to design, implement and test new algorithms for the generation, and adaptation of computational meshes, as well as expressing the finite element method solvers in order to effectively simulate the process of propagation of pollutants described by the advection-diffusion-reaction equations [2]. In particular, the productions of hypergraph grammar [2] express the Rivara's longest-edge refinement algorithm. The expression of the mesh generation algorithm by graph-grammar quarantees the correctness of the mesh and allows for efficient parallelization.

2 Results

In the dissertation, an algorithm for pollution simulations over complicated terrain topography with adaptive finite element method and graph grammar based longest-edge refinement was designed and implemented. The graph-grammar based longest-edge refinement was

Figure 1: Graph grammar based pollution propagation simulation in Lesser Poland. Exemplary production.

employed for modeling the terrain topography and extended to model the generation of the three-dimensional tetrahedral meshes span over the terrain mesh. This graph grammar model was incorporated with the finite element method stabilized with Streamling-Upwind-Petrov-Galerkin (SUPG) method for the non-stationary advection-diffusion-reaction simulations. It allowed running a simulation of the pollution propagation over Lesser Poland area. During the work, it was shown that the graph-grammar based implementation of the longest edge refinement algorithm allows for additional parallelization within a single longest-edge refinement path, thus allowing for extra speedup.

3 Conclusions

The thesis shows how to express, by graph-grammar productions, the longest-edge mesh refinement algorithm for a two-dimensional mesh with triangular elements. The graph-grammar-based algorithm allows for better parallelization than classical Rivara's algorithm. It is also shown how to extend it to the three-dimensional grids and interface with GMRES solver and Crank-Nicolson time integration scheme. The mesh generation algorithm removes all the hanging nodes automatically from the mesh. The stabilized advection-diffusion-reaction solver executed on the computational mesh based on topographic data of Lesser Poland area provides a tool for the pollution propagation simulations. Additionally, a method to include non-regular topographic data into alternating-direction solver with finite difference method was proposed. Also, the graph-grammar based solver was compared with alternating-directions solver indicating that despite linear computational cost of the latter, in its current form it does not allow for mesh adaptation, which makes the graph-grammar based solver more attractive.

References

[1] Rivara M. Algorithms for refining triangular grids suitable for adaptive and multigrid techniques. International journal for numerical methods in Engineering 1984;20:745–756.

[2] Podsiadło K, Serra A. O., Paszyńska A., Montenegro-Armas R., Henriksen I., Paszyński M., Pingali K., Parallel graph-grammar-based algorithm for the longest-edge refinement of triangular meshes and the pollution simulations in Lesser Poland area, Engineering with Computers, 2021;21:3857–3880.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Numerical Study on Thermodiffusive Instabilities in Laminar and Turbulent Hydrogen Flames

Lukas Berger*, Heinz Pitsch

RWTH Aachen University, Templergraben 56, 52056 Aachen, Germany
* e-mail: l.berger@itv.rwth-aachen.de

Abstract: The deployment of hydrogen represents a unique opportunity to decarbonize our energy system. However, its utilization in combustion processes involves several challenges, e.g., lean hydrogen/air flames are prone to thermodiffusive instabilities, which significantly enhance flame speeds and reaction rates and have a leading order effect on the flame dynamics. As the underlying mechanisms lack a detailed understanding, large-scale direct numerical simulations are performed in this work. Key findings comprise the identification and explanation of a largest and smallest intrinsic structure of the unstable flame front corrugations; the quantitative assessment of the thermodiffusive instability mechanism in a large parametric space, linking its effects to fundamental flame properties, and deriving physics-based low-order models; the identification of a synergistic interaction between the thermodiffusive instability and the always prevailing hydrodynamic instability by using a novel modelling approach; and the recognition of synergistic interactions between turbulence and thermodiffusive instabilities, leading to a remarkable four-fold increase of reactivity and a three-fold increase of the flame speed in turbulent flames. Such an increase of flame speed is of utmost engineering relevance for hydrogen-operated combustion devices as it is a key design and model parameter.

Keywords: Hydrogen, Premixed Combustion, Direct Numerical Simulations, Thermodiffusive Instabilities

1. Research Goals

To decarbonize our energy systems, ***hydrogen plays a special role among synthetic fuels as it is carbon-free and very versatile in energy on-demand applications.*** While its utilization bears a huge potential for further optimization of combustion processes, it also involves several scientific and technological challenges. Research needs arise predominantly from the molecular transport and flame properties, which are entirely different from conventional fuels. Hydrogen features a ***significantly higher diffusivity that leads to the onset of thermodiffusive instabilities.*** These instabilities are yet not well understood and ***theoretical models lack an accurate description of them.*** Therefore, a systematic analysis of such instabilities is performed by means of direct numerical simulations (DNS). DNS represent a powerful research tool for model development and analysis as they provide high-fidelity velocity, temperature, and species data, which is typically challenging to obtain simultaneously in experiments. ***The overarching goal is to provide a detailed understanding of the underlying physical processes and to develop predictive combustion***

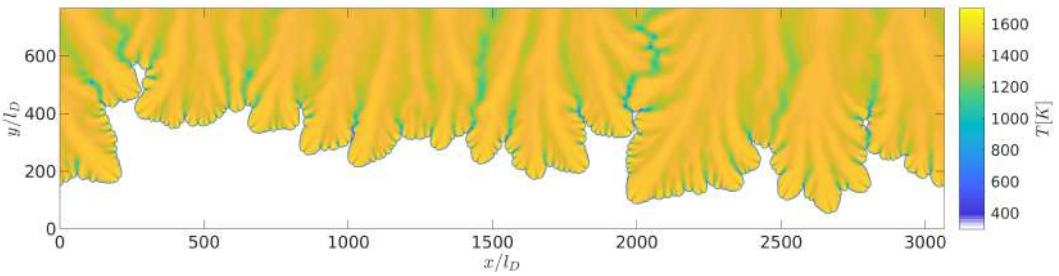


Figure 1. Flame front corrugations in an initially flat hydrogen/air flame ($\phi = 0.4, 298K, 1bar$), leading to a four-fold flame speed increase and super-adiabatic temperatures of up to 200 K.

models that account for the effects of thermodiffusive instabilities. At present, the lack of such models represents a major impediment for the optimization of hydrogen-operated combustion devices.

2. Key Findings

Fig. 1 shows an initially planar hydrogen flame that develops strong corrugations due to the presence of thermodiffusive instabilities, leading to ***a significant four-fold enhancement of the flame consumption speed*** compared to the propagation speed of a flat flame [1]. ***The small-scale cellular flame front corrugations are linked to fundamental growth rates*** obtained from a linear stability analysis [2]. Further, the generation mechanism of the ***large-scale flame fingers, which have been identified as an intrinsic length scale for the first time*** [1]**,** is linked to a ***synergistic interaction of the thermodiffusive instability mechanism with the hydrodynamic instability,*** which always prevails in premixed flames [3]. The propensity of hydrogen/air flames to form thermodiffusive instabilities is studied numerically in a large parametric space of temperature [298-700 K], pressure [1-20 bar], and equivalence ratio [0.4-1.0] relevant to engineering applications. A remarkable six-fold increase of flame speeds is observed for high pressures, low temperatures, and low equivalence ratios, which is ***linked to fundamental flame properties and a low-order model for the flame speed enhancement is derived [4].*** To assess the interactions of thermodiffusive instabilities and turbulence, DNS of a lean hydrogen/air flame in a slot burner configuration at a jet Reynolds number of $Re = 11{,}000$ are performed, which is shown in Fig. 2. ***Turbulence is found to further amplify thermodiffusive instabilities,*** leading to higher flame speeds and super-adiabatic temperatures in the turbulent flame compared to the laminar flame in Fig. 1 [5]. Thermodiffusive instabilities are shown to have ***tremendous effects*** on the flame dynamics in hydrogen/air flames ***with large implications for engineering problems***. Thus, key insights into such instabilities and low-order models for combustor design are proposed in this work.

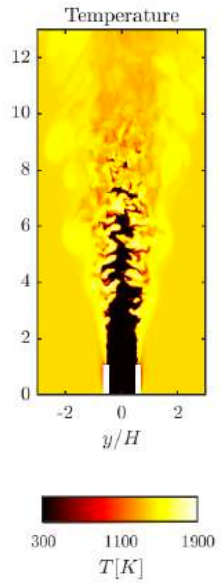


Figure 2. DNS of lean hydrogen/air flame in a slot burner configuration with super-adiabatic temperatures of up to 400 K.

References

[1] L. Berger, K. Kleinheinz, A. Attili, H. Pitsch. Characteristic patterns of thermodiffusively unstable premixed lean hydrogen flames. Proc. Comb. Inst., 37:1879–1886, 2019.
[2] L. Berger, A. Attili, H. Pitsch. Intrinsic instabilities in premixed hydrogen flames: Parametric variation of pressure, equivalence ratio, and temperature. Part 1 - Dispersion relations in the linear regime. Combust. Flame, 240:11935, 2022.
[3] L. Berger, M. Grinberg, B. Jürgens, P.E. Lapenna, F. Creta, A. Attili, H. Pitsch. Flame fingers and interactions of hydrodynamic and thermodiffusive instabilities in laminar lean hydrogen flames. Proc. Combust. Inst., 39, 2022.
[4] L. Berger, A. Attili, H. Pitsch. Intrinsic instabilities in premixed hydrogen flames: Parametric variation of pressure, equivalence ratio, and temperature. Part 2 - Non-linear regime and flame speed enhancement. Combust. Flame, 240:11936, 2022.
[5] L. Berger, A. Attili, H. Pitsch. Synergistic interactions of thermodiffusive instabilities and turbulence in lean hydrogen flames. Combust. Flame, 244:112254, 2022.

VII ECCOMAS Young Investigators Conference

YIC2023

19-21 June 2023, Porto, Portugal

Towards Data-driven Multi-scale Optimization of Thermoplastic Blends: Microstructural Generation, Constitutive Development and Clustering-based Reduced-Order Modeling

Bernardo P. Ferreira*

* School of Engineering, Brown University
Providence RI, United States of America
e-mail: bernardo_ferreira@brown.edu

Abstract:

The present thesis addresses several challenges arising in the development of a state-of-the-art Integrated Computational Materials Engineering (ICME) framework to design and optimize amorphous thermoplastic blends exhibiting a particulate morphology. Without any loss in generality, particular focus is given to PC/ABS, one of the most successful commercial polymer blends composed of Acrylonitrile-Butadiene-Styrene (ABS) particles embedded in a polycarbonate (PC) matrix. Given the high dimensional engineering design space associated with this class of advanced materials, the recent data-driven material design paradigm arises as a promising tool to find optimum process-structure-property-performance bridges. However, unlocking the true potential of such a framework in terms of actual engineering applicability demands the development of powerful computational methodologies -- this is the main driving force of the research endeavor put forth in the present thesis.

A new computational generation method for particle-reinforced materials, coined AMINO (Adaptive Multi-temperature Isokinetic Method), is proposed in a framework of time-driven molecular dynamics [1, 2]. Besides the suitable handling of the intersections between particles through a coupled cell-Verlet list method, AMINO's high efficiency stems from an adaptive (explicit) time integration scheme and a multi-temperature isokinetic thermostat that accelerate the convergence towards a legal configuration. Extensive numerical applications and comparisons with real micrographs demonstrate that AMINO can generate high-fidelity periodic representative volume elements (RVEs) under a broad spectrum of microstructure descriptors.

The recent clustering-based reduced-order modeling framework based on a Lippmann-Schwinger integral equilibrium formulation is thoroughly derived under both infinitesimal and finite strains, and adopted to perform a fast computational homogenization of high-fidelity RVEs. Clustering adaptivity is introduced for the first time in such a framework, enhancing the accuracy of clustering-based reduced-order models (CROMs) by unlocking a dynamic clustering in the prediction stage. A novel adaptive CROM coined Adaptive Self-Consistent Clustering Analysis (ASCA) is shown to accurately capture highly localized plasticity in a particle-reinforced composite while keeping high efficiency [3]. A new finite strain extension of the Self-Consistent Clustering Analysis (SCA) CROM compatible with the multiplicative nature of the deformation gradient is also proposed, being an accurate and robust self-consistent scheme still under investigation.

A visco-elastic-visco-plastic constitutive model is formulated to describe the finite strain nonlinear behavior of amorphous thermoplastics [4]. The constitutive formulation is presented within the framework of thermodynamics of irreversible processes, a highly efficient, fully implicit computational implementation is thoroughly derived, and a two-stage optimization-based calibration procedure is proposed. An excellent agreement between the constitutive model predictions and experimental results is obtained at different temperatures and strain rates for PC, being the distinct stages of the highly nonlinear finite deformation accurately captured. The new model is extended to account for the phenomenon of rubber particle internal

cavitation, which plays a major role in the behavior of rubber-toughened amorphous thermoplastics such as ABS.

Keywords: Computational mechanics, Microstructure generation, Reduced-order modeling, Constitutive modeling, Amorphous thermoplastics

References

[1] Ferreira, B.P., Vila-Chã, J.V.C. and Andrade Pires, F.M., (2021). An adaptive multi-temperature isokinetic method for the RVE generation of particle reinforced heterogeneous materials, Part I: Theoretical formulation and computational framework. Mechanics of Materials, 163.

[2] Ferreira, B.P., Vila-Chã, J.V.C. and Andrade Pires, F.M., (2021). An adaptive multi-temperature isokinetic method for the RVE generation of particle reinforced heterogeneous materials, Part II: Numerical assessment and statistical analysis. Mechanics of Materials, 165.

[3] Ferreira, B.P., Andrade Pires, F.M. and Bessa, M.A., (2022). Adaptivity for clustering-based reduced-order modeling of localized history-dependent phenomena. Computer Methods in Applied Mechanics and Engineering, 393.

[4] Ferreira, B.P., Carvalho Alves, A.F. and Andrade Pires, F.M., (2023). An efficient finite strain constitutive model for amorphous thermoplastics: fully implicit computational implementation and optimization-based parameter calibration. Computers & Structures, 281.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Study of the effect of the tumour microenvironment on cell response using a combined simulation and machine learning approach. Application to the evolution of Glioblastoma.

Jacobo Ayensa-Jiménez[1]

[1] Aragon Institute of Engineering Research (I3A)
Universidad de Zaragoza, Spain.

e-mail: jacoboaj@unizar.es

Abstract: Glioblastoma is the deadliest and most frequent brain tumour. Tumour cells migrate towards oxygenated areas and then proliferate close to the blood vessels, eventually collapsing them and avoiding oxygen supplies. This cyclic behavior is one of the driving forces behind glioma aggressiveness. We present here a computational framework integrating physical knowledge, data obtained from microfluidic devices and machine learning tools for both predicting glioblastoma progression and understanding the metabolic switch between proliferation and migration. The method accurately predicts glioblastoma progression in microfluidic cell cultures and unveils this metabolic switch for different benchmark models, laying the first foundations in the use of data-intensive tools in biomedical engineering and clinical problems for personalized medecine.

Keywords: Physics-Informed Machine Learning, Glioblastoma, Physically-Guided Neural Networks.

1. INTRODUCTION

Glioblastoma (GBM) is the deadliest and most frequent tumour affecting brain tissues [1]. Mathematical models are, in conjunction with experimental data, a valuable tool for a better GBM understanding, prognosis estimation and *in silico* therapy design. However, despite their predictive capacity, these models fail to unravel hidden complex biological processes, masked due to the high non-linearity and coupling of the different phenomena involved.

Recently, a new paradigm is rising in Simulation-Based Engineering and Sciences [2], which aims for incorporating Artificial Intelligence tools to conventional mathematical modelling, though some scepticism exists about their "black box" nature. This lack of explanatory capacity may be supplied by centuries of research, which have resulted in high knowledge about our environment and cannot fall on deaf ears. Cancer processes are not the exception.

In this work, a new approach for analyzing tumour evolution is proposed, combining the use of data and Machine Learning tools with the explanatory capacity of physical models about cancer progression, something nowadays possible thanks to the great advances in cell culture monitoring. A computational framework is built in which GBM evolution is reproduced in microfluidic devices under different experimental configurations, and, more importantly, the metabolic switch from GBM cell migration to proliferation (go-or-grow) is unveiled.

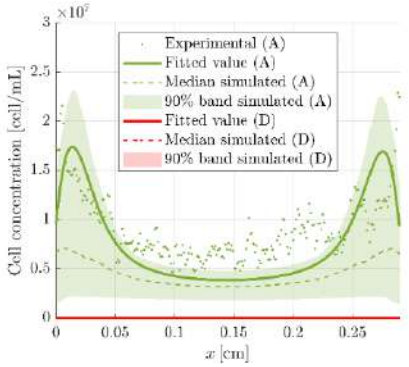
2. METHODS

A computational framework is built for the simulation of GBM in microfluidic devices. The biological system is represented by a set of Partial Differential Equations (PDEs). The go-or-grow switch is encoded in a pair of functions Π_{gr} and Π_{go}, depending on the oxygen level and fitting parameters. Using data from microfluidic devices and a stochastic approach using the concept of *copulae*, the model is calibrated and the go-or-grow explored. This metabolic

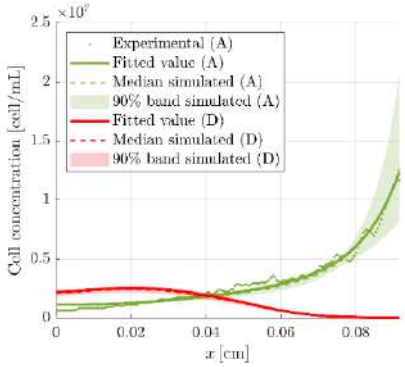
switch is further investigated by means of a special family of Artificial Neural Networks, able to represent non-measurable data and relationships within a consistent physical context.

3. RESULTS

GBM progression is reproduced for different experiments with the parametric approach (Fig. 1). However, there is still important uncertainty in the representation of the go-or-grow. Physically-Guided Neural Networks (PGNN) outperform the parametric approach both for predicting GBM progression and for explaining its nature, when tested over several benchmark models (Fig. 2).

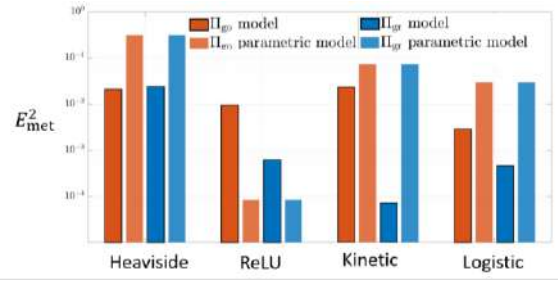


(a) Double pseudopalisade (day 21).

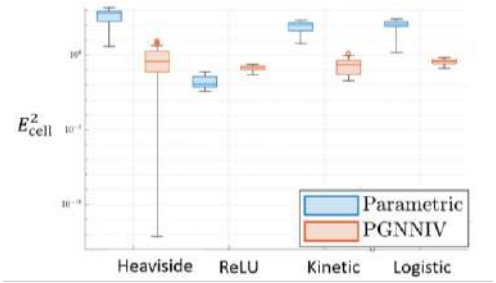


(b) Pseudopalisade (day 6).

Figure 1. Comparizon between the experimental results and the simulations.



(a) Double pseudopalisade (day 21).



(b) Pseudopalisade (day 6).

Figure 2. Errors with the parametric and PGNNIV approach for explaining and predicting GBM progression..

4. CONCLUSIONS

Although good GBM progression predictions are obtained with the parametric approach, PGNN outperform the former in both predictive and explanatory capacity. PGNN learn faster, are less data demanding, and have an extra filtering capacity than conventional NN. A workflow integrating patient-specific data and cell culture monitoring lays the foundations of personalised medicine, letting us glimpse an encouraging future in the fight against GBM.

Acknowledgements

Spanish Ministry of Science and Innovation (project PGC2018-097257-B-C31).

References

[1] Alexander, B. M., et al. (2017). Adult glioblastoma. J. Clin. Oncol., 35(21), 2402-2409.

[2] Karpatne, A., et al. (2017). Theory-guided data science: A new paradigm for scientific discovery from data. IEEE Trans Knowl Data Eng, 29(10), 2318-2331.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modeling the Role of the Stem Cell Niche in Blood Cancer Progression

Thomas Stiehl*

* Institute for Computational Biomedicine - Disease Modeling
RWTH Aachen University, Aachen, Germany &
Department of Science and Environment
Roskilde University, Roskilde, Denmark
e-mail: tstiehl@ukaachen.de

Abstract: Acute myeloid leukemia (AML) is one of the most aggressive cancers. It is driven by cancer stem cells which trigger malignant cell expansion and impairment of healthy blood cell formation. There is evidence that cancer stem cells and blood forming (hematopoietic) stem cells compete for supportive micro-environments, so-called stem cell niches. We propose mathematical models helping to understand how stem cell competition affects AML clinical course and patient prognosis. The proposed models provide new insights into the problem of prognostic stratification and interpretation of patient samples.

Keywords: Hematopoietic stem cell, cancer stem cell, stem cell niche, acute myeloid leukemia, prognosis, competition, mechanistic computational modeling, ordinary differential equations, disease modeling

1 Introduction

Tissue stem cells drive homeostasis and regeneration. Unlike other cell types they can perform a (potentially) unlimited number of divisions and give rise to multiple types of specialized cells. Due to their ability to self-renew, the stem cell population persists throughout the life of an organism. The tissue stem cells responsible for blood cell formation are referred to as hematopoietic stem cells (HSCs). HSCs are located in specialized micro-environments in the bone marrow, so-called stem cell niches, which they require to preserve their function.

AML is driven by leukemic stem cells (LSCs) [1]. The LSCs interfere with the HSC niche and give rise to the heterogeneous malignant cell bulk. The malignant cell expansion eventually leads to impairment of healthy blood cell formation. Due to its limited accessibility, our knowledge about the human HSC niche and its role in AML is limited.

2 Approach and Results

We consider a set of non-linear ordinary differential equation models [2, 3, 4, 5] to better understand the interaction of HSCs, LSCs and the niche. The models account for important feedback mechanisms of the hematopoietic system and for the competition of healthy and malignant cells. We combine model analysis and computer simulations to investigate how processes in the stem cell niche impact on AML progression.

In agreement with clinical observations [6] the models [4, 5] assume that HSCs and LSCs compete for spaces in a joined stem cell niche. The progeny arising from stem cell division attempt to conquer a niche space, either by adhering to a previously empty space or by

dislodging a stem cell from the niche (LSCs can dislodge HSCs and vice versa). Stem cells finding no niche space or stem cells dislodged from the niche are assumed to lose stemness.

Model simulations suggest that the LSC division rate and the probability quantifying dislodgement of HSCs by LSCs have a major impact on the speed of disease progression. We use measurements of the leukemic cell burden in the bone marrow (blast fraction) and of HSC counts at the time of AML diagnosis [6] to fit the model to individual patients. Based on the estimated LSC proliferation rate and HSC dislodgement probability we subdivide patients into prognostic groups. For the patients considered in [6] this approach provides additional information compared to the clinically used (i.e., cytogenetic) risk scoring.

More detailed models of cellular interactions accounting for detachment, attachment, division, differentiation and self-renewal of the stem cells [2, 3] identify high self-renewal and high niche attachment rates as factors increasing the competitive advantage of LSCs over HSCs. Simulations suggest that the malignant cell burden in the stem cell niche potentially differs from the malignant cell burden measured in blood or whole bone marrow samples.

3 Conclusions

The combination of computational modeling and patient data suggests that properties of leukemic stem cells might impact on the clinical course of AML. Computational modeling can help to understand how processes in the stem cell niche are linked to disease progression and thus contribute to prognostic stratification of AML patients.

References

[1] Bonnet D, Dick JE. Human acute myeloid leukemia is organized as a hierarchy that originates from a primitive hematopoietic cell. Nat Med. 1997;3(7):730-7.

[2] Pedersen RK, Andersen M, Skov V, Kjaer L, Hasselbalch HC, Ottesen JT, Stiehl T. HSC niche dynamics in regeneration, pre-malignancy and cancer: Insights from mathematical modeling. Stem Cells. 2022; doi: 10.1093/stmcls/sxac079. Epub ahead of print.

[3] Pedersen RK, Andersen M, Stiehl T, Ottesen JT. Mathematical modelling of the hematopoietic stem cell-niche system: Clonal dominance based on stem cell fitness. J Theor Biol. 2021;518:110620.

[4] Stiehl T, Wang W, Lutz C, Marciniak-Czochra A. Mathematical Modeling Provides Evidence for Niche Competition in Human AML and Serves as a Tool to Improve Risk Stratification. Cancer Res. 2020;80(18):3983-3992.

[5] Stiehl T. Using mathematical models to improve risk-scoring in acute myeloid leukemia. Chaos. 2020;30(12):123150.

[6] Wang W, Stiehl T, Raffel S, Hoang VT, Hoffmann I, Poisa-Beiro L, Saeed BR, Blume R, Manta L, Eckstein V, Bochtler T, Wuchter P, Essers M, Jauch A, Trumpp A, Marciniak-Czochra A, Ho AD, Lutz C. Reduced hematopoietic stem cell frequency predicts outcome in acute myeloid leukemia. Haematologica. 2017;102(9):1567-1577.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Phenotypic plasticity as a vehicle for tumour progression: joint insights from experimental data and mathematical models.

Ortega-Sabater Carmen[*,1]

[*,1] Mathematical Oncology Laboratory (MOLAB), Department of Mathematics
University of Castilla-La Mancha
Ciudad Real, Spain e-mail: carmen.ortegasabater@uclm.es

Abstract: Phenotypic diversity plays a major role in tumour development and patients outcome. Phenotypic plasticity acts a source of diversity in cancer, beyond genetic mutations. We propose a mathematical modeling framework for stochastic changes affecting proliferation rate, based both on a reaction-advection-diffusion model and a discrete model. We provide experimental validation in a non-small cell lung cancer cell line (NCI-H460). We consider the role of additional variables on cell growth, such as growth factors seggregation and cell-to-cell interactions. We use an analogous approach to assess the role of chromosomal instability in aneuploid subtypes of childhood B-acute lymphoblastic leukemia using real data from patients. Using a discrete simulator we discuss how, within a certain range, chromosomal instability increase the chances that the cells reach a fitter phenotype shaping patients response, as observed in real-life patients.

Keywords: Evolutionary dynamics, cancer, cell proliferation, phenotypic plasticity, chromosomal instability, partial differential equations, mathematical models, discrete simulator, B-acute lymphoblastic leukemia.

1 Introduction

Evolutionary dynamics comprises all the changes in time at many different biological scales, ranging from individuals to complete ecosystems. In the light of evolution, tumour progression has often been explained by looking at the somatic changes of cancer cells. However, it is extensively known that cancer evolution goes far beyond genetic changes. Tumour heterogeneity takes places at different levels, including the genome, transcriptome, proteome and subsequently, the phenome, or the phenotypic distribution affecting a certain cell trait. We wanted to assess the impact of stochastic fluctuations affecting cell traits as a source of phenotypic diversity and how they may affect tumour progression.

2 Methods and results

Firstly, we focused on cell proliferation and we approached this general problem from a theoretical and computational point of view. We proposed a discrete stochastic model describing the growth dynamics of an initially clonal population of tumour cells. Due to stochastic changes, these cells may end up showing different proliferation rates, giving rise to a phenotypic distribution in proliferation. We derived the balance equation into a reaction-advection-diffusion model:

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial \rho^2} - v\frac{\partial n}{\partial \rho} + \rho n - \mu n \tag{1}$$

where $n = n(\rho, t)$ denotes the cell density function. The first term in (1) accounts for the fluctuations on the proliferation rate ρ which occur with a constant phenotypic diffusion coefficient (D), which is necessarily greater than zero. The second term represents the drift in proliferation with a velocity v. Finally, we included cell proliferation and apoptosis in the third and fourth term, respectively. Our simulations revealed that phenotypic distribution broads in time and cell population showed a faster-than-exponential growth dynamics. From this reaction-advection-diffusion model a complete set of ordinary differential equations for the evolution in time of total cell number (N), mean proliferation rate ($\langle\rho\rangle$) and for the variance of the phenotypic distribution ($\langle\sigma^2\rangle$) These three ODEs constitute an exactly solvable model, allowing us to obtain an explicit expression for the standard deviation ($\langle\sigma\rangle(t)$), the mean proliferation ($\langle\rho\rangle(t)$) and total population ($N(t)$). We used these results to validate our hypothesis experimentally in a non-small cell lung cancer cell line (NCI-H460). Detailed information is provided in [1].

Although we focused until this point on cell proliferation, phenotypic plasticity affects every cell trait and it has a direct impact on the behaviour of the cell as a whole. Although it is generally hidden behind epigenetics, gene regulation and other molecular processes, the biological basis of phenotypic plasticity is hard to define or delimit. Understanding it as a substrate for evolution to occur may be a good starting point. This rationale was later on applied to real patients data. We addressed the role of chromosomal instability on the development of different clinical phenotypes in patients affected by childhood B-acute lymphoblastic leukemia (B-ALL) [2]. We developed a discrete simulator which incorporates parameters based on single-cell karyotyping data at diagnosis (sequenced by NGS) and after B-ALL progression in PDX models. Mitotic deffects, missegregation rates, dynamics of blast fraction in peripheral blood and proteomics data were also taken into account. We worked on the definition of a contribution to fitness value for each individual chromosome. We addresed the trade-off between cell diversity and cell viability.

3 Conclusions

Our results suggest that phenotypic transitions sustaining continuous proliferation rate increase could be spontaneous and take place even in the absence of evolutionary pressures. Additionally, chromosomal instability acts as a source of variation for tumour cells, giving them the chance to reach fitter karyotypes and resembling on *virtual* patients outcome what has been observed in real patients.

References

[1] Ortega-Sabater, C., F. Calvo, G., Dinić, J. et al. Stochastic Fluctuations Drive Non-genetic Evolution of Proliferation in Clonal Cancer Cell Populations. Bull Math Biol 85, 8. 2023. https://doi.org/10.1007/s11538-022-01113-4.

[2] Molina O, Abad MA, Solé F, Menéndez P. Aneuploidy in Cancer: Lessons from Acute Lymphoblastic Leukemia. Trends Cancer. 7(1):37-47. 2021. doi: 10.1016/j.trecan.2020.08.008.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Modelling the impact of intra-tumour heterogeneity on radiotherapy outcomes

Giulia Celora*, Helen Byrne† and Panos Kevrekidis‡

* Department of Mathematics
University College London (UCL)
London, UK
e-mail: g.celora@ucl.ac.uk

† Wolfson Centre for Mathematical Biology,
Mathematical Institute, University of Oxford
Oxford, UK

‡ Department of Mathematics and Statistics,
University of Massachusetts Amherst
Amherst, US

Abstract: In cancer, treatment failure and recurrence of disease have been linked to the diverse makeup of tumors, where cells with varying characteristics (such as sensitivity to treatment) coexist. In this talk, I will present a structured-population model to describe the evolution of tumour heterogeneity in a slice of tissue which is oxygenated from the boundary by a vessel and exposed to radiation treatment. The model consists of a system of coupled non-local partial differential equations that links the phenotypic evolution of tumour cells to the local oxygen levels and treatment. Using a combination of analytical and numerical techniques to investigate model predictions, I will show how the model can be used to inform general principle for the design of radiotherapy protocols that are more effective than standard of care regimens commonly applied in the clinic.

Keywords: evolutionary dynamics, cancer stem cells, radiotherapy

1 Introduction

Failure of cancer treatments is often associated to intra-tumour heterogeneity. While current treatments are effective in killing the bulk of the tumour, it is the presence of small subpopulation of (stem-like) resistant cells that are eventually responsible for relapse. Experimental evidence suggests that cues from the tumour microenvironment, such as hypoxia (*i.e.*, abnormally low oxygen levels), can drive tumour cells to transition towards an aggressive, treatment-resistant phenotype (a stem-like state). Mathematical modelling can help in understanding the spatio-temporal evolution of intra-tumour heterogeneity under the influence of various environmental factors and how this then reflects pm disease progression and treatment outcomes.

2 Predicting the impact of intra-tumour heterogeneity on radiotherapy outcomes

In our recent publication [1], we propose a novel mathematical model, structured by phenotype and space, to investigate the impact of spatial variation in oxygen levels on a tumour's phenotypic composition and growth dynamics in the presence and absence of radiotherapy.

The proposed model consists of a system of coupled non-local and non-linear partial differential equations that links the phenotypic evolution of tumour cells to the local oxygen levels and radiotherapy treatment. As shown in [1], in the absence of treatment and for biologically realistic values of the model parameters, the system has two non-negative stable steady states which can be mapped to a "tumour-extinction" and a "tumour-invasion" scenario.

In this talk, I will focus on how we can use the insights gained from the analysis of the long-term behavior of model solutions to design treatment strategies that are more effective than standard protocols currently used in clinics. A key insight from the model is the importance of monitoring a tumor's burden and its phenotypic composition to predict treatment outcomes. In particular, we find that a successful treatment strategy must jointly control the tumor burden and the prevalence of resistant stem-like cells. Leveraging numerical simulations, I will demonstrate how this can be accomplished by modifying standard radiotherapy schedules to include "treatment holidays". By comparing model-informed protocols with standard of care, we find that the former can lead to the successful eradication of more aggressive tumors for which standard of care fails. I will conclude the talk by discussing the limitations of our modeling framework and the challenges that arise when considering translating model predictions to the clinic.

References

[1] G. L. Celora, H. M. Byrne, P.G. Kevrekidis. *Spatio-temporal modelling of phenotypic heterogeneity in tumour tissues and its impact on radiotherapy treatment.* Journal of Theoretical Biology (556), 2023, doi:10.1016/j.jtbi.2022.111248

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

On optimal temozolomide scheduling for slowly growing gliomas

Berta Segura-Collar[1,2*], Juan Jiménez-Sánchez[3,4*], Ricardo Gargini[1,2*], Miodrag Dragoj[5], Juan M. Sepúlveda[2], Milica Pesic[5], María A. Ramírez[1], Luis E. Ayala-Hernández[3], Pilar Sánchez-Gómez[1#], Víctor M. Pérez-García[3,4#]

[1]Neurooncology Unit, Instituto de Salud Carlos III (ISCIII)
Madrid, Spain

[2]Instituto de Investigaciones Biomédicas I+12, Hospital 12 de Octubre
Madrid, Spain

[3]Mathematical Oncology Laboratory (MOLAB), University of Castilla-La Mancha (UCLM)
Ciudad Real, Spain

[4]IMACI, University of Castilla-La Mancha (UCLM)
Ciudad Real, Spain

[5]Department of Neurobiology, University of Belgrade
Belgrade, Serbia

[*]Co-first authors
[#]Co-senior authors

Abstract: Temozolomide (TMZ) is part of the standard of care in the management of glioblastoma (GBM), and is commonly used in low-grade gliomas (LGG). In this work, we explored alternative TMZ schedules to assess whether they outperform standard of care for gliomas. Agent-based mathematical models fed with either mouse or patient data were developed for *in-silico* studies of therapy optimization. The experimental data used to confirm the results were mouse glioma models, human GBM U251 cells immobilized in alginate microfibers, and patient data from the TCGA/TCIA public databases and TOG clinical study. Slow-growth "virtual" murine GBMs benefited from increasing TMZ dose separation *in-silico*. In line with the simulation results, improved survival, reduced toxicity, lower expression of resistance factors, and reduction of the tumor mesenchymal content were observed in experimental models subject to long-cycle schedules. Tissue analysis after long-cycle TMZ treatments revealed epigenetically driven changes in tumor phenotype. Virtual clinical trials provided support for implementation methods in human patients. In conclusion, we provided *in-silico*, *in-vitro* and *in-vivo* evidence supporting that TMZ administration schedules with increased time between doses may reduce toxicity, delay the appearance of resistances and lead to survival benefits in slowly-growing GBMs.

Keywords: *In-silico* clinical trial, Mathematical oncology, Optimal drug scheduling, Temozolomide resistance, Tumor phenotype, Cellular automata

1 Introduction

Temozolomide is an oral alkylating agent commonly used in low-grade gliomas, and as the standard of care in the management of glioblastomas, due to its favorable toxicity profile [1]. However, its moderate effect, together with the resistance induced by MGMT methylation status [2,3], have

spurred the search for ways to increase the effect of this drug. While there is plenty of research looking for better scheduling strategies, no rationale has been found supporting alternative administrations. Based on temozolomide short half-life, with the aim of depleting intracelular MGMT, dose-dense regimens have been proposed and tested even in clinical trials [4], to no avail. In this work, we provide evidence suggesting that protracted temozolomide therapy may be beneficial in terms of survival, resistance and toxicity, even outperforming standard therapy schemes.

2 Extended abstract content

We conducted in-silico, in-vitro and in-vivo studies to find optimal drug schedules based in long-cycle schemes outperforming standard ones in terms of survival, resistance and toxicity. Agent-based mathematical models fed with either mouse or patient data were developed for the in-silico studies [5]. The experimental test beds used to confirm the results were: mouse glioma models obtained by retroviral expression of EGFR-wt/EGFR-vIII in primary progenitors from p16/p19 ko mice and grown in-vitro and in-vivo in orthotopic allografts [6], and human glioblastoma U251 cells immobilized in alginate microfibers. The patient data used to parametrize the model were obtained from the TCGA/TCIA databases and the TOG clinical study.

Slow-growth 'virtual' murine gliomas benefited from increasing temozolomide dose separation in-silico. In line with the simulation results, improved survival, reduced toxicity, lower expression of resistance factors and reduction of the tumor mesenchymal component were observed in experimental models subject to long-cycle treatment, particularly in slowly-growing tumors. Tissue analysis after long-cycle temozolomide treatments revealed epigenetically-driven changes in tumor phenotype, which could explain the reduction in glioma growth speed. In-silico trials provided support for implementation methods in human patients.

3 Conclusions

In-silico, in-vitro and in-vivo studies show that temozolomide administration schedules with increased time between doses may reduce toxicity, delay the appearance of resistances and lead to survival benefits mediated by changes in the tumor phenotype in gliomas [7].

References

[**1**] Stupp R, Mason WP, van den Bent MJ, et al. Radiotherapy plus concomitant and adjuvant temozolomide for glioblastoma. N Engl J Med. 2005; 352(10):987-996.
[**2**] Hegi ME, Diserens AC, Gorlia T, et al. MGMT gene silencing and benefit from temozolomide in glioblastoma. N Engl J Med. 2015; 352(10):997-1003.
[**3**] Rabé M, Dumont S, Álvarez-Arenas A, et al. Identification of a transient state during the acquisition of temozolomide resistance in glioblastoma. Cell Death Dis. 2020; 11(1):19.
[**4**] Gilbert MR, Wang M, Aldape KD, et al. Dose-dense temozolomide for newly diagnosed glioblastoma: a randomized phase III clinical trial. J Clin Oncol. 2013; 31(32):4085-4091.
[**5**] Jiménez-Sánchez J, Martínez-Rubio Á, Popov A, et al. A mesoscopic simulator to uncover heterogeneity and evolutionary dynamics in tumors. PLoS Comput Biol. 2021; 17(2): e1008266.
[**6**] Segura-Collar B, Garranzo-Asensio M, Herranz B, et al. Tumor-derived pericytes driven by EGFR mutations govern the vascular and immune microenvironment of gliomas. Cancer Res. 2021.
[**7**] Segura-Collar B, Jiménez-Sánchez J, Gargini R, et al. On optimal temozolomide scheduling for slowly growing glioblastomas. Neuro-Oncology Advances, 2023; 4(1): vdac155.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

A multiscale model for combined therapy effects on glioma progression

Conte Martina*, Surulescu Christina†, Dzierma Yvonne §, and Knobe Sven‡

* Department of Mathematical Sciences "G. L. Lagrange"
Politecnico di Torino
Torino, Italy
e-mail: martina.conte@polito.it

† Felix-Klein-Zentrum für Mathematik
Technische Universität Kaiserslautern
Kaiserslautern, Germany
e-mail: surulescu@mathematik.uni-kl.de

§ Department of Radiotherapy and Radiation Oncology
Saarland University Medical Centre
Homburg/Saar, Germany
e-mail: Yvonne.Dzierma@uks.eu

‡ Department of Radiotherapy and Radiation Oncology
Saarland University Medical Centre
Homburg/Saar, Germany
e-mail: Sven.Knobe@uks.eu

Abstract: A multiscale model for glioma spread in brain tissue under the influence of vascularization is proposed to investigate and compare various therapy approaches. Precisely, these involve radio- and chemotherapy in a concurrent or adjuvant manner together with anti-angiogenic therapy affecting the vascular component of the system. We assess tumor growth and spread on the basis of DTI data and we apply our model to real glioma patient data, showing the effects of a space-dependent radiotherapy plan.

Keywords: Multiscale glioma modeling; interplay with VEGFs and blood vessels; combined treatment efficacy.

1 Introduction

Glioma is the most prevalent, aggressive, and invasive subtype of primary brain cancer, characterized by rapid cell proliferation and great infiltration capacity [1]. Its infiltrative spread is strongly related to very poor patient survival prognosis, considering the difficulty to properly assess tumor margins for effective treatment. Tumor growth and migration in the brain is a highly complex phenomenon, influenced by a multitude of intrinsic and extrinsic factors at different spatial and temporal scales. Here, we propose a kinetic-based approach for the description of glioma progression with a specific focus on the influence of the brain vasculature on therapeutic effects.

2 Extended abstract content

The basis for kinetic descriptions of glioma and endothelial cell (ECs) dynamics can be found in [2]. Here, we extend those settings upon considering a more detailed description at the microscopic level. Starting from the subcellular dynamics, we consider tumor receptor binding to anisotropic brain tissue and blood vessels together with the dynamics of vascular endothelial growth factor (VEGF) receptors located on the EC membrane. The tumor evolution, in fact, takes advantage of the patient-specific anisotropic brain structure, in particular white matter tracts and blood vessels, which influences the direction of cell migration. The relevance of these specific structures in the overall tumor evolution motivates the need of developing personalized treatment planning, which should include such characteristics. Moreover, at both the microscopic and mesoscopic level, we include in the description different terms characterizing the effects of radio-, chemo-, and anti-angiogenic therapy. This allows us to derive a macroscopic system of equations describing tumor-ECs dynamics, together with VEGFs, healthy, and necrotic tissues evolution [3].
We numerically test our model in several scenarios, particularly focusing on the effects that different treatment combinations can have on the evolution of the neoplasia. In particular, we analyze the difference on the long-term tumor progression of different time administration of the anti-angiogenetic. Moreover, taking advantage of the real patient data we had access to, we observe the effects of a space-dependent radiotherapy plan of both the neoplastic and healthy tissue, obtaining qualitatively reasonable results. Altogether, these results show how multiscale models seem to offer an adequate frame for studying the effects of various therapy ansatzes and have the potential to investigate a great variety of therapeutic scenarios (of which we showed here just a few examples) in an unprecedented complexity and accuracy.

References

[1] Berens M E, Giese A. ... those left behind. Biology and oncology of invasive glioma cells, Neoplasia, 1999;1(3):208–19.

[2] Conte M, Surulescu C. Mathematical modeling of glioma invasion: acid- and vasculature mediated go-or-grow dichotomy and the influence of tissue anisotropy, Appl. Math. Comput., 2021; 407:126305.

[3] Conte M, Surulescu C. Mathematical modeling of glioma invasion and therapy approaches via kinetic theory of active particles, Accepted in Math. Models Methods Appl. Sci.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Bridging the gap between individual cell movement and macroscopic cancer invasion models

Dimitrios Katsaounis*, Mark A.J. Chaplain† and Nikolaos Sfakianakis‡

*School of Mathematics and Statistics
University of St Andrews
St Andrews, United Kingdom
e-mail: dk204@st-andrews.ac.uk

†School of Mathematics and Statistics
University of St Andrews
St Andrews, United Kingdom
e-mail: majc@st-andrews.ac.uk

‡School of Mathematics and Statistics
University of St Andrews
St Andrews, United Kingdom
e-mail: n.sfakianakis@st-andrews.ac.uk

Abstract: Invasion of the surrounding tissue is a key aspect of cancer growth and spread involving a coordinated effort between cell migration and matrix degradation, and has been the subject of mathematical modelling for almost 30 years. In this current work we address a long-standing question in the field of cancer cell migration modelling. Namely, identify the migratory pattern and spread of individual cancer cells, or small clusters of cancer cells, when the macroscopic evolution of the cancer cell colony is dictated by a specific partial differential equation (PDE). The results presented have been accepted for a publication.

Keywords: Cancer invasion, multiscale modelling, hybrid continuum-discrete, coupled partial and stochastic partial differential equations.

Cancer invasion is a complex process involving numerous interactions between the cancer cells and the extracellular matrix (ECM) (cf. the tumour microenvironment) facilitated by matrix degrading enzymes. Active cell migration (both individual and collective) and increased/excessive proliferation enable the local spread of cancer cells into the surrounding tissue or to secondary locations via blood or lymphatic vessels i.e., metastasis or metastatic spread. An overview of the core aspects of invasion can be found in [2]. From a mathematical modelling perspective, cancer invasion has been a topic of interest for almost 30 years with a range of approaches and techniques being used, and an overview can be found in the recent review paper [5].

The processes of solid tumour growth and cancer invasion have been typically described in the mathematical oncology literature using deterministic, macroscopic models of partial differential equations (PDEs). These models include interactions with the tumour microenvironment, leading to complex mathematical descriptions. One of the key modelling premises is that the solid tumour is comprised of a large number of cancer cells – indicatively around 10^9 cells in $1\ \text{cm}^3$ of tumour tissue. It is hence evident that a macroscopic description of the tumour is better suited for mathematical—if not for biological—investigations.

On the other hand, the mathematical description of cancer cells migrating at the individual

cell level allows for a higher degree of biological realism [4]. Consequently this introduces a large system of (usually) stochastic differential equations (SDEs) that are neither amenable to mathematical analysis nor straightforward computational simulation unlike many macroscopic models. However, it is clear that constructing models that capture the motion of individual cancer cells, directed by a drift force, that diffuse into their environment, will give a more accurate representation of their biological behaviour.

Nonetheless it is understood that these two mathematical descriptions should be interchangeable with intrinsically identifiable and correlated cell migration properties. In this work by Katsaounis et al. (in press) [3] we shed light on the relation between macroscopically described cancer invasion models [1, 6] and the migratory properties of the individual cancer cells. We show that the usual heuristic understanding of the diffusion and advection terms of the PDE being one-to-one responsible for the random and biased motion of the solitary cancer cells, respectively, is not precise. On the contrary, we show that the drift term of the correct SDE scheme that dictates the individual cancer cell migration, should account also for the divergence of the diffusion of the PDE. We support our claims with a number of numerical experiments and computational simulations. We hence offer a bridge between the two mathematical descriptions that allows us to scrutinise and accordingly improve the biological tractability of the macroscopic cancer invasion models, and the mathematical analysis at the individual cell level.

References

[1] L.C. Franssen, N. Sfakianakis, and M.A.J. Chaplain. A novel 3d atomistic-continuum cancer invasion model: In silico simulations of an in vitro organotypic invasion assay. J. Theor. Biol., 522:110677, 2021.

[2] D. Hanahan and R.A. Weinberg. The hallmarks of cancer. Cell, 100:57–70, 2000.

[3] D. Katsaounis, M.A.J. Chaplain, and N. Sfakianakis. Stochastic differential equation modelling of cancer cell migration and tissue invasion. Journal of Mathematical Biology, in press.

[4] C.K. Macnamara, A. Caiazzo, I. Ramis-Conde, and M.A.J. Chaplain. Computational modelling and simulation of cancer growth and migration within a 3d heterogeneous tissue: The effects of fibre and vascular structure. Journal of Computational Science, 40:101067, 2020.

[5] N. Sfakianakis and M.A.J. Chaplain. Mathematical modelling of cancer invasion: A review. In T. Suzuki, C. Poignard, M. Chaplain, and V. Quaranta, editors, Methods of Mathematical Oncology. MMDS 2020. Springer Proceedings in Mathematics & Statistics, vol 370, pages 153–172. Springer, Singapore, 2021.

[6] N. Sfakianakis, A. Madzvamuse, and M.A.J. Chaplain. A hybrid multiscale model for cancer invasion of the extracellular matrix. Multiscale Modeling & Simulation, 18(2):824–850, 2020.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Growth dynamics of brain metastases

Ocaña-Tienda, Beatriz [1*], Pérez-Beteta, Julián[1] Ortiz de Mendivil, Ana[2], Asenjo, Beatriz[3], Albillo, David[4], Pérez-Romasanta, Luís[5], Arana, Estanislao[6] and Pérez-García, Víctor M.[1]

[1] Mathematical Oncology Laboratory
University of Castilla-La Mancha, Ciudad Real, Spain
e-mail*: Beatriz.Ocana@uclm.es

[2] Sanchinarro University Hospital, HM Hospitales, Madrid, Spain
[3] Hospital Regional Universitario de Málaga, Málaga, Spain
[4] MD Anderson Cancer Center, Madrid, Spain
[5] Salamanca University Hospital, Salamanca, Spain
[6] Fundación Instituto Valenciano de Oncología, Valencia, Spain

Abstract: Scaling laws were used in this study to characterize the growth dynamics of brain metastases (BM), the most common intracranial tumour in adults, when they were subjected to various treatments. The scaling law exponent beta was used as a growth factor to describe the dynamics. We have demonstrated that the growth patterns of radiation necrosis, an adverse event occurring after irradiation, and tumour recurrence differ, which may aid in their differentiation in clinical settings. We have also used mathematical models that incorporate elements of the tumour biology and inflammatory response to support our findings, and the results are consistent with our observations.

Keywords: Mathematical oncology, brain metastases, scaling laws, radiation necrosis

1 Introduction

The interplay of complex biological processes in a huge number of individual cells existing in varying environments leads to tumor development. In straightforward experimental models, it has been demonstrated that mathematical growth laws can accurately predict the longitudinal dynamics of tumour growth [1, 2]. Results regarding the development of human malignancies in patients, however, are limited. In order to identify growth laws for untreated and recurrently treated brain metastases (BMs), our work mined a large dataset of 1133 BMs with longitudinal imaging follow-up.

After radiation therapy (RT) for BMs, radiation necrosis (RN) is a common side effect. Because RN and progressive disease (PD) seem identical on magnetic resonance images (MRIs), it might be challenging to discern them apart. Previous theoretical studies anticipated that RN would experience a quicker, although temporary, growth dynamics after RT, but no study has used patient data to support that hypothesis. We hypothesize that recurrent BMs and RN events might be distinguished using lesion size time dynamics derived from growth laws matched with data from consecutive volumetric measurements on MRIs.

2 BM longitudinal growth dynamics

The Von-Bertalanffy equation [3]

$$\frac{dV}{dt} = \alpha V^{\beta}, \tag{1}$$

has been proven recently to accurately captures the longitudinal dynamics of growing human tumors [4]. It has been argued, and confirmed with data from human cancers, that malignant tumors with heterogeneous clonal composition have exponents $\beta > 1$.

Three patient groups were examined: (i) patients with BMs that were growing untreated, (ii) patients with BMs that were recurring after radiation therapy, and (iii) patients who were undergoing chemotherapy (CT) but who did not get any specific BM treatment. For untreated BMs ($N = 10$), the fitted individual exponents' median value was $\beta = 1.59$. For BMs growing under CT, the median growth exponent was $\beta = 0.64$ ($N = 16$). We found $\beta = 0.72$ ($N = 23$) for BMs that continued to grow following radiation therapy (RT). Last but not least, among those who underwent RT and were subjected to CT, we obtained $\beta = 0.68$ ($N = 33$).

3 Radiation Necrosis

Due to the quicker dynamics of inflammatory processes, growth exponents in patients with RNs were shown to be significantly bigger than those in patients with PD. Between the two groups, there were statistically significant differences ($p < 0.001$). The capacity of the growth law exponent to classify the events was supported by the ROC curve (AUC = 0.76).

4 Conclusions

In summary, our analysis of a large set of BM data revealed a constant acceleration of growth caused by Darwinian competition between various tumour subpopulations. Recurrent BMs showed slower growth, which is consistent with a decrease in tumour heterogeneity driven on by the treatment. Additionally, growth law exponents derived from sequential longitudinal MRIs following RT can be used as an additional tool in the differential diagnosis between RN and progressing disease.

References

[1] Benzekry, S. et al., Classical mathematical models for description and prediction of experimental tumor growth. *PLoS Comput Biol.* **10**(8), e1003800 (2014).

[2] West, J,., & Newton, P.K. , Cellular interactions constrain tumor growth. *Proc Natl Acad Sci U S A.*. **116**(6), 1918-1923 (2019).

[3] Von Bertalanffy L., Quantitative laws in metabolism and growth. *Q Rev Biol.* **32**(3), 217-231 (1957).

[4] Pérez-García, V.M. et al. , Universal scaling laws rule explosive growth in human cancers. *Nature Phys.* **16**, 1232–1237 (2020).

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Advances in the use of machine learning techniques to accelerate the topology optimisation process on structural problems

A. Martínez-Martínez[1*], E. Nadal[1], J.M. Navarro-Jiménez[1], O. Allix[2], J. J. Ródenas[1]

[1] Instituto de Ingeniería Mecánica y Biomecánica (I2MB)
Universitat Politècnica de València, Valencia, Spain
email: anmar29a@etsid.upv.es, ennaso@upvnet.upv.es, jonaji@upv.es, jjrodena@mcm.upv.es

[2] ENS Paris-Saclay, CNRS, LMT Laboratoire de Mcanique et Technologie
Universit Paris-Saclay, 91190, Gif-sur-Yvette, France
email: olivier.allix@ens-paris-saclay.fr

Keywords: Machine Learning, Multi-scale Topology Optimisation, Finite Element Analysis, Artificial Neural Network.

Abstract

In recent years, the use of methods from the artificial intelligence field in topology optimisation schemes has been an active area of research [1]. These machine-learning-based models have mainly been applied to create direct optimised designs or accelerate these procedures. One of the main challenges in this field is improving the multiscale resolution of structural problems.

This study presents a new methodology to accelerate the topology optimisation process at the mesoscale by using neural networks. The multiscale topology optimisation process involves solving a global topology optimisation process for material distribution. Then, the macro problem is divided into cells or regions where the resolution is improved by applying mesoscale topology optimisation in each cell. Since the number of cells can be significant, the computational cost of such an algorithm is expensive. Then, taking advantage of the repeated structure of the cells, a neural network-based topology optimisation algorithm is trained to obtain the topology of each cell at a small computational cost.

In this talk, we present the architecture of the Artificial Neural Network used for the mesoscale topology optimisation process, considering its limitations and performance in the selected problems. Finally, we will present this methodology's preliminary results and the potential applications fields as topology-optimised infill designs that can be used in several applications as prostheses or any mechanical design of light structures.

Acknowledgements

The authors gratefully acknowledge the support of Ministerio de Educación (FPU19 /02103) and Generalitat Valenciana (Prometeo/2021/046 and CIAICO/2021/226).

References

[1] Woldseth Id, R. v, Id, N. A., Andreas Baerentzen Id, J., & Id, O. S. (2022). On the use of Artificial Neural Networks in Topology Optimisation. https://doi.org/10.48550/arxiv.2208.02563

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Artificial intelligence methods for preliminary sizing of aircraft structures

Gómez Ordoño, Daniel[*] and Llamas Sandín, Raúl Carlos[†]
[*] Simulation Methods Department
Airbus Operations
Madrid, Spain
e-mail: daniel.gomez-ordono@airbus.com

[†] Future Projects Department
Airbus Operations
Madrid, Spain
e-mail: raul.c.llamas@airbus.com

Abstract: This study involves the development of a weight optimisation method for simply supported composite thin walled structures under buckling and strength constraints, to be used in the preliminary design of aircraft structures. The paper involves two parts: First, a neural network is trained with finite element results to predict the initial buckling of the plates under combined compression and shear loads, obtaining a relative error lower than 1% in the majority of laminates. The second part, involves the development of an optimisation method in the Julia language, with computational speed as a priority. A greedy approach is followed to obtain an optimal database of stacking sequences for a range of compression and shear loads. All stacking sequences in the database satisfy blending constraints, that is, all plies in the thinner laminates have continuity throughout the thickest laminates in the structure. Different strategies are presented and compared and the methods are validated by comparison with an exhaustive search approach.

Keywords: laminate, optimisation, neural network, buckling

1. INTRODUCTION

Preliminary sizing of composite structures is one of the main necessities when studying new designs in the aeronautics industry. New configurations require a constant analysis of the failure modes and the strength of the structure, needing updates after each iteration. A preliminary sizing method must necessarily have a fast execution speed while reaching reasonable accuracy. The method proposed in this document aims to optimise execution speed while keeping enough accuracy for a preliminary design stage. Specifically, the method will focus on finding an optimised laminate database in terms of weight for a range of compression and shear loads, which assures compatibility amongst the laminates so that the structure can be manufactured.

To obtain the desired computational speed, a neural network is trained with buckling results from a finite element method (FEM) model so that the buckling analysis during the optimisation process does not highly penalise the computational time.

In 2019, X. Liu proposed in his thesis [1] an optimisation method based on lamination parameters which is highly representative of the state of the art of this approach. This method consists of two stages: first, optimal lamination parameters and thickness are found with VICONOPT software. In the second stage, a branch and bound method is used to find the stacking sequence which matches the first lamination parameters and satisfies the constraints. Other approaches of existing methods have been developed by [2], where the optimisation algorithm works with the ply orientations directly instead of lamination parameters. Irisarri et al. [3] introduced a new concept, stacking sequence tables, in which each number of plies is

given an associated laminate, adding plies from the thinnest laminate to assure compatibility, and the location and order of ply drop-offs is determined. Adams et al. in 2004 [4] introduced an optimisation method in which the optimal compatible laminates were obtained by, given a thick guide laminate, progressively deleting contiguous innermost or outermost plies with a genetic algorithm. Yang et al. in 2016 [5] improved this method by allowing any ply to be deleted instead of heavily restricting the design space by only deleting innermost or outermost plies.

Compared to the previous methods, the main difference is that this paper presents a greedy algorithm, looking for an improvement in efficiency and a simplification of the way lay-up constraints are introduced. The use of neural networks to substitute FEM will also be integrated in the method to avoid the time consuming analysis while keeping most of the accuracy.

2. NEURAL NETWORK TRAINING

2.1. Input parameters

As stated in the introduction, the neural network is trained with buckling solutions for simply supported composite panels using FEM under combinations of compression and shear loads. For the choice of input parameters, the priority is to find the optimal input parameters which have enough influence in the problem for the neural network to understand and be able to distinguish different cases. In reference [6], it is proven that, for infinitely long plates, compression and shear buckling coefficients can be expressed as a function of the buckling parameter, which expressions are included in equations (1). The aspect ratio ϕ of the plate is another input parameter, taking into account geometry effects. Lastly, the relation between shear buckling ratio and compression buckling ratio is needed to predict the results in a combined compression and shear case.
For the prediction objective, a non-dimensional parameter representing the ratio between the critical load obtained by FEM and an approximate analytical buckling load, so that the neural network only needs to learn the first-order error in the problem due to the hypotheses in the analytical model.

$$\alpha = \sqrt[4]{\frac{D_{11}}{D_{22}}},\ \beta = \frac{D_{12}+2D_{66}}{\sqrt{D_{11}D_{22}}},\ \gamma = \frac{D_{16}}{\sqrt[4]{D_{11}^3 D_{22}}},\ \delta = \frac{D_{26}}{\sqrt[4]{D_{11}D_{22}^3}} \quad (1)$$

2.2. Results

A representative example of the results obtained is shown in Figure 1 for a pure compression case. The relative error obtained compared to FEM is under 0.3 % for almost every laminate in a validation database which includes more than 60000 laminates with different geometries and stacking sequences.

3. OPTIMISATION RESULTS

The optimisation for a given range of compression and shear loads outputs a database of compatible laminates such as the one presented in Figure 2. In this case, iterations start from laminate (-45, 45, 0, 90)S, and the algorithm adds plies as the load increases ensuring compatibility and satisfying buckling and strength restrictions. Thickness of the resultant laminates are compared with an exhaustive search approach which proves that the relative error is highly dependent on the problem but can be reduced to values under 5 % in many load ranges with the appropriate methods and input parameters.

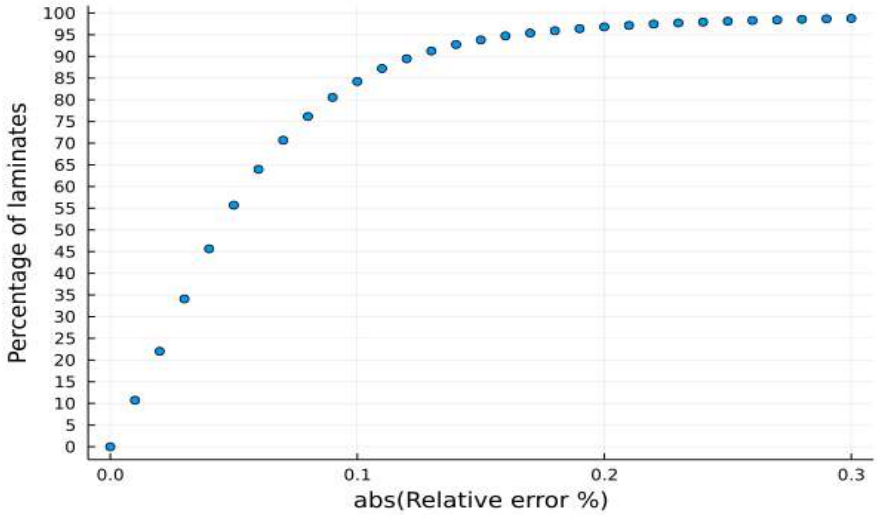


Figure 1. Relative error to FEM in pure compression neural network predictions vs. percentage of laminates

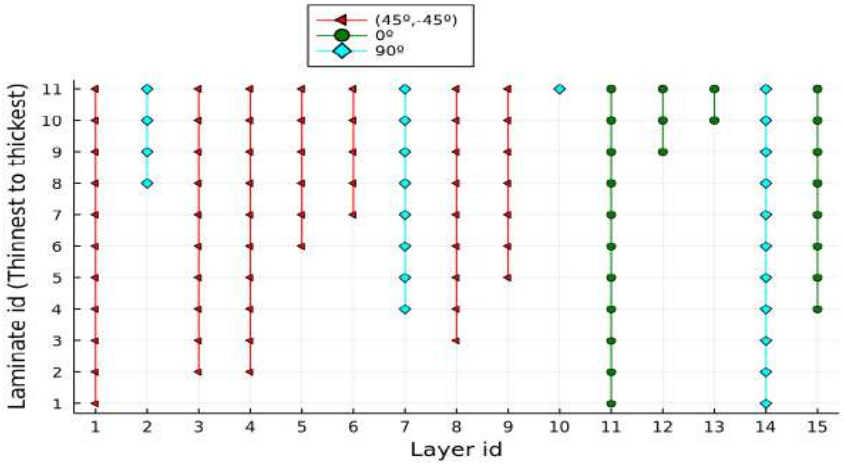


Figure 2. Output example of the optimisation algorithm. Layer "1" represents the outer layer and layer "15" the middle layer. Laminate 1 corresponds to the least restrictive load case and and laminate 11 to the most. All laminates are symmetric.

4. Conclusions

In the neural network training process, input parameters for the training to be successful were proposed and analysed. Instead of designing the neural network to directly predict buckling critical loads, it was checked that taking advantage of analytical buckling equations which obtained approximate results and adjusting them to FEM results made the neural network correctly understand the patterns in the problem and distinguish the input parameters to produce its output. Optimisation methods results have shown that, as long as compatibility is required, there is not a large potential of improvement and greedy algorithm, despite not entirely exploring the design space, finds in most cases the best compatible solution in a short run-time. Comparison with an exhaustive search method has allowed to analyse the load states and geometries where the error was happening and to introduce alternative methods to provide more flexibility to the user.

References

[1] Xiaoyang Liu. Optimum Design of Composite Structures using Lamination Parameters. PhD thesis. Cardiff University, 2019.

[2] Sachin Shrivastava et al. Optimal design of fighter aircraft wing panels laminates under multi-load case environments by ply-drop and ply-migrations 2019. Composite Structures 207 pp. 909–922.

[3] F.-X. Irisarri et al. Optimal design of laminated composite structures with ply drops using stacking sequence tables 2014. Composite Structures 107 pp. 559-569.

[4] David B. Adams et al. Genetic algorithm optimization and blending of composite laminates by locally reducing laminate thickness 2004. Advances in Engineering Software 35.1 pp. 35–43.

[5] Junbo Yang et al. Optimal design of blended composite laminate structures using ply drop sequence 2016.Composite Structures 135, pp. 30–37.

[6] Michael P. Nemeth. Buckling behavior of long symmetrically laminated plates subjected to combined loadings. NASA technical paper 1992.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Polymer creep modulus prediction by leveraging CAMPUS database and gradient boosting

Lobato, Héctor[12*]; Cernuda, Carlos[3]; Arriaga, Aitor[1]; Zulueta, Kepa[1]; Burgoa, Aizeti[1]

[1] Leartiker S. Coop.
Markina Xemein, Spain
* e-mail: hlobato@leartiker.com

[2] University of the Basque Country (UPV/EHU)
Leioa, Spain

[3] Electronics and Computing Dept.
Mondragon University
Arrasate-Mondragon, Spain

Abstract: The prediction of creep behavior plays a critical role in the design of plastic parts and products intended for prolonged use. Creep modulus, which describes the relationship between stress and strain that a material experiences over time, is important for determining the long-term performance of engineering materials. However, due to the time-consuming and resource-intensive nature of testing for this property, we sought to investigate the potential utility of machine learning techniques as an alternative approach. To accomplish this, we downloaded and curated a dataset comprising more than 400 different polymer grades using CAMPUS online free database. Following the best practices in materials informatics, we obtained accurate assessments of the models' ability to generalize to new data. Using the LightGBM gradient boosting framework, we obtained the most accurate predictions, demonstrating that machine learning algorithms can be useful to estimate the creep modulus of materials given a sufficiently large database. In this ongoing research, we believe predictions can be improved by injecting physics into the models.

Keywords: machine learning, creep behavior, polymers, materials informatics, material property prediction

1 Introduction

Creep behavior prediction is crucial when designing plastic parts and products that will be used for long periods. Creep is a slow and continuous deformation of solid materials under prolonged load or stress below the yield strength of the material [1]. Polymeric materials suffer especially from this effect due to their viscoelastic response and can face a significant tensile modulus reduction even under ambient operating conditions (unlike metallic materials).

Creep modulus (CM) refers to the relation between the stress and strain that a material experiences over time, and gives us information about the long-term performance of engineering materials. However, testing for this property can be difficult due to its dependence on temperature and applied load and the long and resource-consuming testing times required. In this work, we explore the use of machine learning (ML) to predict creep behavior, akin to the past work of other researchers [2, 3], but for a wider range of material grades.

2 Methods

2.1 Database creation

The main bottleneck for the development of data-driven algorithms in R&D workflows is obtaining the data, virtually in any field but especially in science. To circumvent this costly data-obtaining process, we used the online database CAMPUS [4]. We downloaded all available information on the materials containing the evolution of CM with time at different applied loads and temperatures.

These CM values had been obtained following the ISO 899-1 standard [5], recording strains for the times of 1 h, 10 h, 10^2 h, 10^3 h, and 10^4 h for five stress levels and a maximum of six temperatures. Our dataset, obtained after cleaning and organizing the data, comprises more than 450 materials and over 5000 rows that include CM at various times for specific load and temperature combinations, as well as the corresponding material properties.

2.2 Feature engineering

Our primary objective was to identify the most effective predictors of CM from materials properties, but missing data hindered the accuracy of the models. As a result, we opted to temporarily forego using material properties, instead utilizing CM values at early times to predict values at longer durations, in addition to applied load and temperature. Furthermore, we discovered that utilizing the ratios between consecutive CMs over time, instead of the proper values, improved predictions.

2.3 Model selection

In pursuit of accurate predictions, we employed various ML regression models of increasing complexity, including decision trees, random forests, and gradient boosting techniques. We found that the former [6] were the most suitable, at the expense of interpretability. We selected the LightGBM algorithm [7] because of its superior computational performance.

We developed models for distinct targets, such as CM at 10^2 h using values at 1 h and 10 h as features, or CM at 10^3 h inputting the values at 1 h, 10 h, and 10^2 h. To tune the models, we split the data following the best practices in materials informatics [8] by avoiding the use of identical or similar materials in different splits simultaneously. To accurately evaluate the models' generalization capabilities, we employed double (or nested) cross-validation, which addresses the issue of over-optimism present in standard k-fold cross-validation [9].

3 Conclusions

All models achieved high accuracy, with R^2 values mostly above 0.99 across all test sets in the nested cross-validation. We showed that, by exploiting a substantial database, gradient boosting techniques can bypass the most time-consuming experimental tests and obtain precise estimates of the long-term CM of materials. We will investigate ways to incorporate physics into the models to improve the accuracy and trustworthiness of the predictions.

References

[1] Evans RW, Wilshire B. Creep of metals and alloys. United States: IMM North American Pub. Center,Brookfield, VT; 1985.

[2] Yang C, Ma W, Zhong J, Zhang Z. Comparative Study of Machine Learning Approaches for Predicting Creep Behavior of Polyurethane Elastomer. Polymers 2021;13:1768. https://doi.org/10.3390/polym13111768.

[3] Wang J, Fa Y, Tian Y, Yu X. A machine-learning approach to predict creep properties of Cr–Mo steel with time-temperature parameters. J Mater Res Technol 2021;13:635–50. https://doi.org/10.1016/j.jmrt.2021.04.079.

[4] CAMPUSplastics n.d. https://www.campusplastics.com/ (accessed October 26, 2022).

[5] 1ISO 899-1:2017. ISO n.d. https://www.iso.org/standard/72819.html (accessed January 13, 2023).

[6] Friedman JH. Greedy function approximation: A gradient boosting machine. Ann Stat 2001;29. https://doi.org/10.1214/aos/1013203451.

[7] Ke G, Meng Q, Finley T, Wang T, Chen W, Ma W, et al. LightGBM: A Highly Efficient Gradient Boosting Decision Tree. Proc. 31st Int. Conf. Neural Inf. Process. Syst., Red Hook, NY, USA: Curran Associates Inc.; 2017, p. 3149–57.

[8] Wang AY-T, Murdock RJ, Kauwe SK, Oliynyk AO, Gurlo A, Brgoch J, et al. Machine Learning for Materials Scientists: An Introductory Guide toward Best Practices. Chem Mater 2020;32:4954–65. https://doi.org/10.1021/acs.chemmater.0c01907.

[9] Fearn T. Double Cross-Validation. NIR News 2010;21:14–5. https://doi.org/10.1255/nirn.1194.

VII ECCOMAS Young Investigators Conference
YIC2023
19-21 June 2023, Porto, Portugal

Topology optimization of an exhaust bracket

Madina Odriozola, Iñaki[*]; Zulueta Uriondo, Kepa[*]

[*] Leartiker S.Coop.
Markina-Xemein, Spain
e-mail: kzulueta@leartiker.com imadina@leartiker.com

Abstract:

Lightweight is one of the most important aspect of automotive industry and consequently several metallic parts of the cars have been replaced by composites. Apart from changing the materials, parts have been developed using different techniques and topology optimization is one of most used. In this research an experimental work have been done to develop a car exhaust bracket using topology optimization. The aim was to replace a metallic bracket with a Sheet Moulding Compound (SMC) material made part. The material has been moulded and different mechanical tests have been done to characterize the mechanical properties at different temperatures and fibre orientations. PTC Creo design software have been used to create the different geometries where the design spaces, geometrical constraints and volume reductions were defined and required load case was applied. With the most suitable geometries, structural analyses have been carried out using Abaqus software in order to validate the designs. Can be concluded that this methodoly of creating geometries using topology optimization and carrying out the validation in a CAE software is useful for product development.

Keywords: Conceptual design, SMC, topology optimization, product development.

1. INTRODUCTION

In the highly competitive automotive industry, component weight reduction is becoming increasingly important. More and more metal components are being replaced by reinforced polymeric materials. One of the most widely used polymeric materials in the automotive industry is Sheet Moulding Compound (SMC), which consists of a thermoset polymeric matrix reinforced with glass or carbon fibre. SMC is a technology that involves moulding a part by compressing it and applying heat through a press. It is widely used in the automotive industry because it allows small or large parts to be formed at a fairly fast manufacturing rate. These materials are even being used in components where they have to withstand high load conditions or in high temperature applications, such as an exhaust bracket.

Structural optimisation plays an important role in the development of a component. There are several methodologies that can be used for the development of a component, but, one of the most powerful one is the topology optimization. Topology optimization tools run close-loop structural simulation loops of a initial design for identifying the functional areas and stress-carrying-zones within the part. This allows the algorithms to remove material from non-critical areas in order to achive certain volume or weight reduction on the part.

2. EXPERIMETAL WORK

In this work an experimental study has been carried out in order to redesign a metal exhaust bracket by SMC material-made part, using topological optimization to develop a suitable geometry.

2.1. Initial geometry

In the following image can be seen the original metallic exhaust bracket:

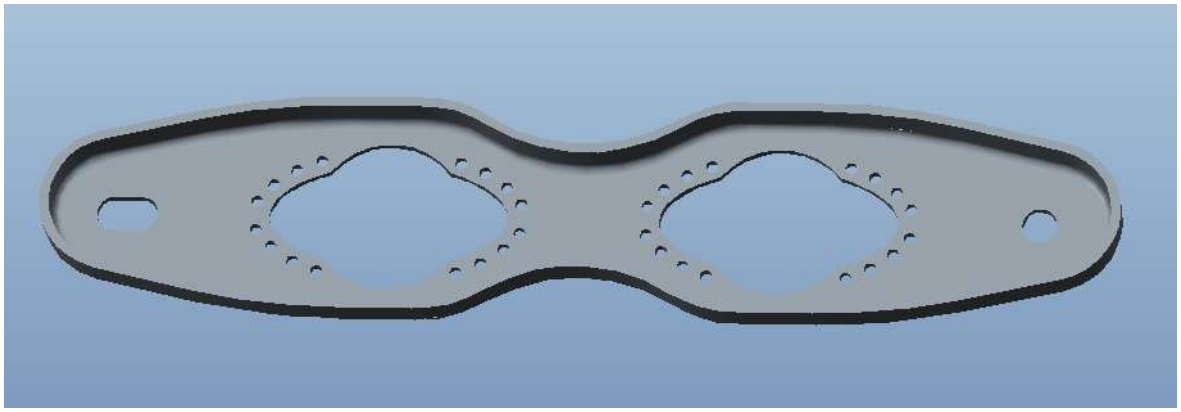


Figure 1. Original metallic exhaust bracket.

This component has two pieces of silicone that are over-injected into the two central holes of it. In the following image can be observed the final assembly of the component with both silicone parts:

Figure 2. Original metallic exhaust bracket with 2 over-injected silicone parts.

This bracket is tied up with two screws to the structure of the vehicle, has to withstand a vertical static force of 660 N and work in a constant 130ºC environment.

2.1. Optimized geometry

Once the working conditions are defined, an initial geometry has been designed in the PTC Creo software. The system then generates an optimised geometry for the set conditions. Based on the structural analysis, a volume reduction objective has been defined and geometries have been optimised according to the load conditions. After generating an

optimized geometry in Creo, Abaqus software have been used for the structural validation. In the following image can be observed a structural analysis of an optimized geometry:

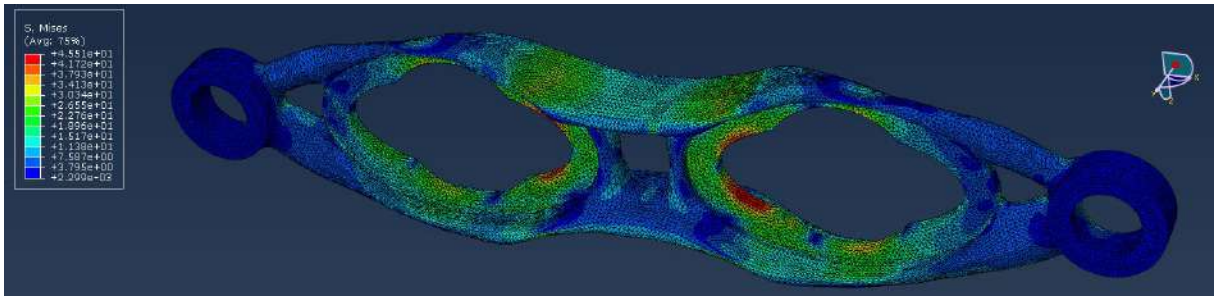
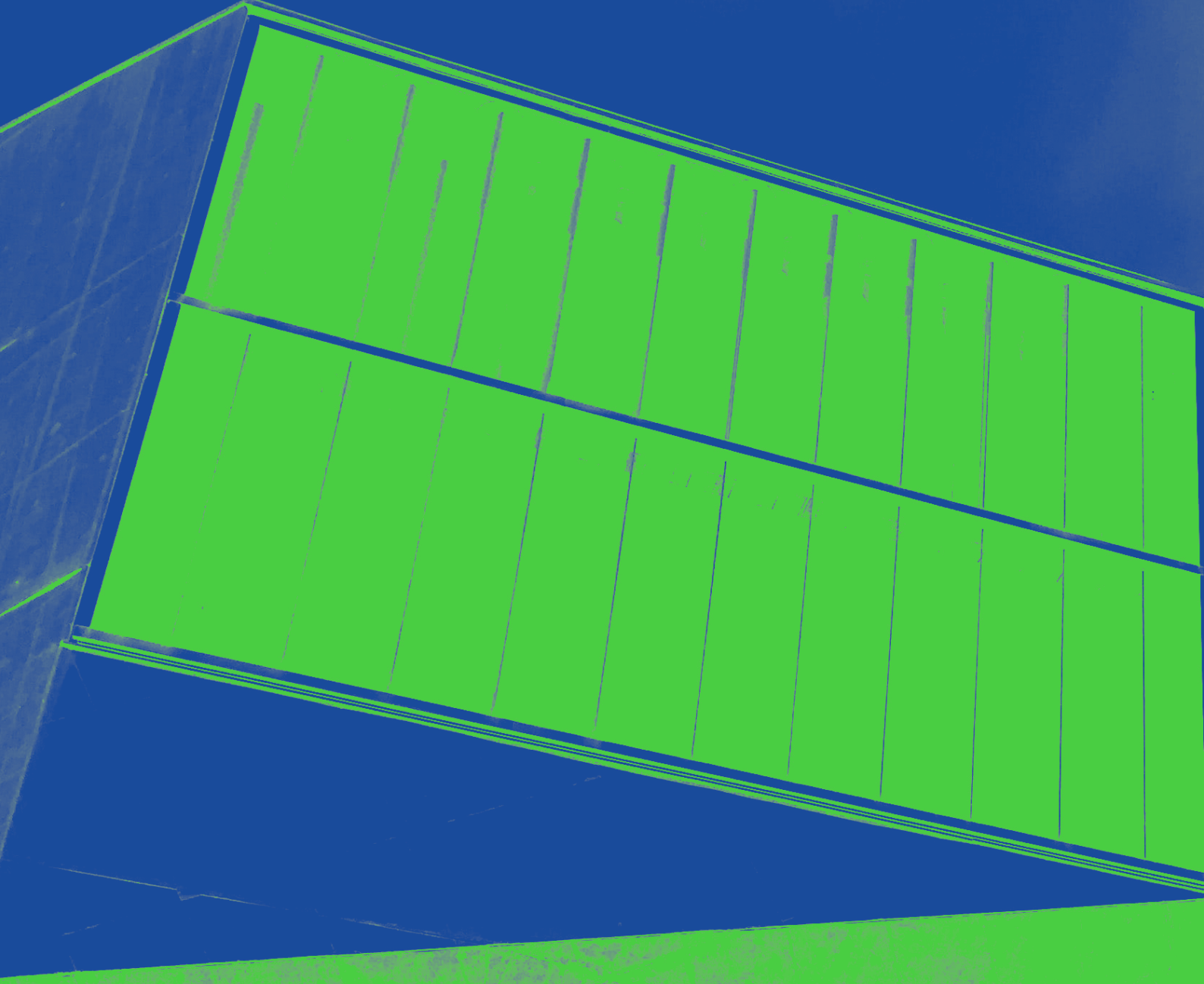


Figure 3. Abaqus structural analysis of an optimized bracket geometry.

3. Conclusions

The main conclusion of tis work is that this methodology of generatimg geometries using topology optimization and validating using a CAE software is useful for product development. It has been shown in this research that topology optimization is an useful technique for conceptual design generation of plastic parts for metallic parts substitution allowing the identification of stress paths and critical areas on the design spaces of the parts.



SPONSORS · GOLD

Vestas®

mathematics
an Open Access Journal by MDPI

SPONSORS · BRONZE

construction materials
an Open Access Journal by MDPI

SN

NASHERO

INSTITUTIONAL SPONSORS

INSTITUTO DA CONSTRUÇÃO

CONSTRUCT

laeta
laboratório associado

Santander
UNIVERSIDADES

Porto.