New Challenges in Data-Driven Modeling

GAMM AG Data Workshop 2019

May 06-07, 2019

RWTH Aachen University

Contents

1 Scope

GAMM ACTIVITY GROUP DATA-DRIVEN MODELING AND NUMERICAL SIMULATION OF MICROSTRUCTURED MATERIALS

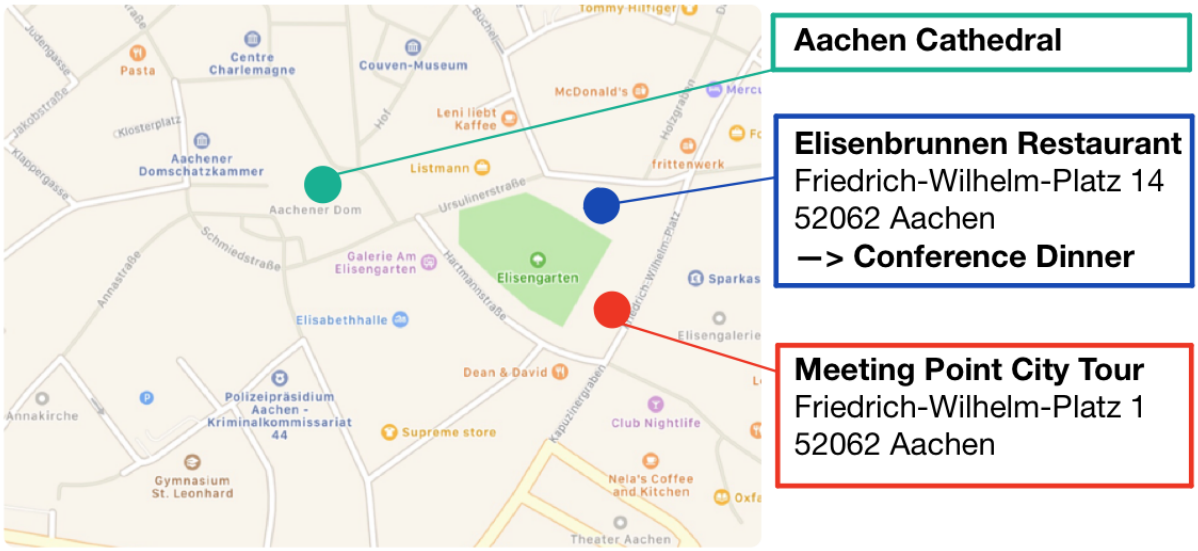
The GAMM AG Data aims at coordinating the activities of the members of the International Association of Applied Mathematics and Mechanics (GAMM) in the field of data-based modeling, simulation and analysis in the context of microstructured materials.
In recent years, the field of imaging based experimental methods has experienced significant technological improvements. For instance, the quality and the speed of computed tomography based imaging techniques have advanced considerably, while at the same, X-ray computed tomography devices are now available in many research facilities. By virtue of the obtained three-dimensional voxel images, microstrucutres of modern natural and artificial materials can be analyzed and used directly in numerical simulations. Incorporating three-dimensional microstructure data is, however, highly non-trivial from a numerical point of view. Special data processing techniques that are able to operate on billions of unknowns, are required. Developing algorithms and data processing techniques for processing three-dimensional data sets constitute major topics of the GAMM AG Data. Innovative image processing techniques for automatic phase segmentation and microstrucutre reconstructions are of equal importance.

2 Objectives

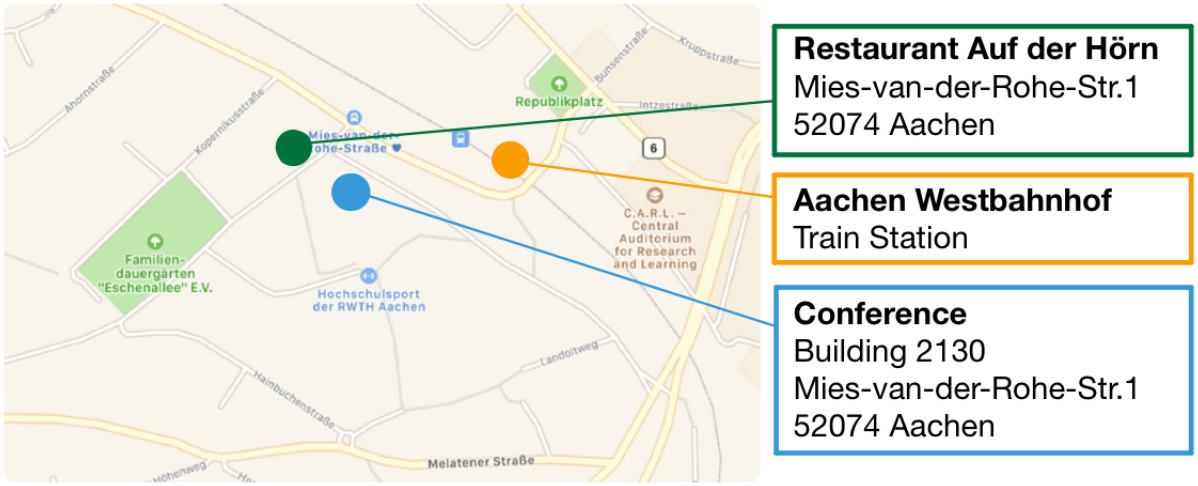
- To discuss the state of the art and recent trends in computational and experimental research.
- To plan AG Data activities.
- Explore possible collaborations with DGM.

3 Practical information

Below you will find all relevant places conference activities taking place. The buses 11, 14, 21, 44, 350 and SB63 will bring you from main station to station Elisenbrunnen. In case you are attending the conference directly, we recommend to take a train to Aachen Westbahnhof.



Monday's and Tuesday's lunch will be at Restaurant "Auf der Hörn", which is less than 100 m from the conference venue.



4 List of participants

Organizers

Stefanie Reese	RWTH Aachen University, Institute of Applied Mechanics (IFAM)
	stefanie.reese@rwth-aachen.de
Felix Fritzen	University of Stuttgart, Institute of Applied Mechanics
	fritzen@mechbau.uni-stuttgart.de
Robert Eggersmann	RWTH Aachen University, Institute of Applied Mechanics (IFAM)
	robert.eggersmann@ifam.rwth-aachen.de
Steffen Kastian	RWTH Aachen University, Institute of Applied Mechanics (IFAM)
	steffen.kastian@rwth-aachen.de

Participants

Frederic E. Bock	Institute of Materials Research, Materials Mechanichs, HZ-Geesthacht
	frederic.bock@hzg.de
Stefan Diebels	Applied Mechanics, Saarland University, Saarbrücken
	s.diebels@mx.uni-saarland.de
Felix Ernesti	Institute of Engineering Mechanics, KIT, Karlsruhe
	felix.ernesti@kit.edu
Mauricio Fernàndez	Institute of Applied Mechanics, University of Stuttgart
	mauricio.fernandez@mechbau.uni-stuttgart.de
Steffen Freitag	Institute for Structural Mechanics, Ruhr University Bochum
	steffen.freitag@sd.rub.de
Johannes Goerthofer	Institute of Engineering Mechanics, Karlsruhe Institute of Technology
	johannes.goerthofer@kit.edu
Markus Hillgaertner	Department of Continuum Mechanics, RWTH Aachen University
	hillgaertner@km.rwth-aachen.de
Martin Huschka	Fraunhofer EMI
	Martin.Huschka@EMI.Fraunhofer.de
Ralf Jänicke	Department of Applied Mechanics, Chalmers University of Technology
	ralf.janicke@chalmers.se
Benjamin Klusemann	Institute of Materials Research, Materials Mechanichs, HZ-Geesthacht
	benjamin.klusemann@leuphana.de
Tim Korzeniowski	Institute of Solid Mechanics, University Siegen
	tim.korzeniowski@uni-siegen.de
Jannick Kuhn	Robert Bosch GmbH
	Jannick.Kuhn@de.bosch.com
Oliver Kunc	Institute of Applied Mechanics (CE), University of Stuttgart
	kunc@mechbau.uni-stuttgart.de
Adrien Leygue	Institute de Recherce en Génie civil et Mécanique, Ecole Centrale Nantes, France
	adrien.leygue@ec-nantes.fr
Kevin Linka	Department of Continuum and Materials Mechanics, Hamburg University of Technology
	kevin.linka@tuhh.de
Julian Lißner	Institute of Applied Mechanics, University of Stuttgart
	lissner@mechbau.uni-stuttgart.de

André Mielke	Institute of Mechanics, Structural Analysis, and Dynamics, University of Stuttgart
	andre.mielke@isd.uni-stuttgart.de
Selina Neuhaus	Applied Mechanics, Saarland University, Saarbrücken
	selina.neuhaus@uni-saarland.de
Michael Ortiz	Division of Engineering and Applied Science, California Institute of Technology
	ortiz@aero.caltech.edu
Auriane Platzer	Institute de Recherce en Génie civil et Mécanique, Ecole Centrale Nantes, France
	auriane.platzer@ec-nantes.fr
Tim Ricken	Institute of Mechanics, Structural Analysis, and Dynamics, University of Stuttgart
	tim.ricken@isd.uni-stuttgart.de
Katrin Schulz	Institute of Applied Materials (IAM-CMS), Karlsruhe Institute of Technology
	katrin.schulz@kit.edu
Jörg Unger	Bundesanstalt für Materialforschung und -prüfung
	joerg.unger@bam.de
Oliver Weeger	Department of Mechanical Engineering, Technische Univerität Darmstadt
	weeger@cps.tu-darmstadt.de
Matthias Wieler	Robert Bosch GmbH
	matthias.wieler@de.bosch.com

5 Timetable

Monday, 06.05.2019

10:00 - 11:30	**City tour Aachen** (Elisenbrunnen - Tourist information)	
12:00	**Lunch** ("Auf der Hörn" - Mies-van-der-Rohe-Straße 10)	
12:50 - 13:00	**Opening** (Mies-van-der-Rohe-Straße 1 - Room 511)	
13:00 - 13:25	Session 1	**Felix Ernesti**, M. Schneider, T. Böhlke Institute of Engineering Mechanics, KIT, Karlsruhe *An FFT based micro mechanics solver for brittle fracture.*
13:25 - 13:50		**Johannes Görthofer**, M. Schneider, A. Hrymak, T. Böhlke Institute of Engineering Mechanics, KIT, Karlsruhe *Computational homogenization of Sheet Molding Compound composites based on generated unit cells.*
13:50 - 14:15		**Oliver Kunc**, F. Fritzen Efficient Methods for Mechanical Analysis, University of Stuttgart *Homogenization for large deformations based on silico data.*
14:15 - 14:40	**Coffee break** (Room 309a)	
14:40 - 15:05	Session 2	**Frederic Bock**, R. Aydin, C. Cyron, N. Huber, S. Kalidindi, B. Klusemann Institute of Materials Research, Materials Mechanichs, HZ-Geesthacht *Machine learning and data mining applications for identification of key dependencies across multiple scales in continuum materials mechanics*
15:05 - 15:30		**Katrin Schulz**, S. Kreis, N. Magino, H. Trittenbach Institute of Applied Materials, KIT Karlsruhe *Data-driven stress prediction for failure analysis.*
15:30 - 15:55		**Steffen Kastian**, S. Reese Institute of Applied Mechanics, RWTH Aachen *Usage of data to create efficient surrogate models and to train low-rank approximations.*
15:55 - 16:20	**Coffee break** (Room 309a)	
16:20 - 16:45	Session 3	**Steffen Freitag** Institute for Structural Mechanics, Ruhr University Bochum *Artificial neural networks for the modeling of the consitutive behavior of materials.*
16:45 - 17:10		**Kevin Linka**, M. Hillgärtner, C. Cyron Department of Continuum and Materials Mechanics, Hamburg University of Technology *Deep learned (micromechanical) constitutive modeling of hyperleastic materials.*
17:10 - 17:35		**Marcus Hillgärtner**, K. Linka, M. Itskov Department of Continuum Mechanics, RWTH Aachen *Towards deep learned constitutive models based on two-dimensional strain fields.*
17:35 - 18:15	Discussion (e.g. NFDI, AG Data activities)	
19:00	Conference Dinner	

Tuesday, 07.05.2019

8:45 - 9:10	Session 4	**Robert Eggersmann**, T. Kirchdoerfer, S. Reese, L. Stainier, M. Ortiz Institute of Applied Mechanics, RWTH Aachen *A general approach for model-free data-driven inelasticity.*
9:10 - 9:35		**Auriane Platzer**, M. Ortiz, L. Stainier, A. Leygue Institute de Recherce en Génie civil et Mécanique, Ecole Centrale Nantes, France *Data-driven finite strain elasticity.*
9:35 - 10:00		**Tim Korzeniowski**, K. Weinberg Institute of Solid Mechanics, University Siegen *Towards data driven finite element analysis.*
10:00 - 10:30		**Michael Ortiz** Division of Engineering and Applied Science, Caltech, Pasadena, USA *Model-free Data-Driven Computing.*
10:30 - 11:00	**Coffee break** (Room 309a)	
11:00 - 11:25	Session 5	**Andre Mielke**, T. Ricken Institute of Mechanics, Structural Analysis, and Dynamics, University of Stuttgart *Artificial Neural Networks as Surrogate Models.*
11:25 - 11:50		**Julian Lißner**, F. Fritzen Univerity of Stuttgart *Data-Driven Microstructure Property Relations.*
11:50 - 12:15		**Oliver Weeger** Department of Mechanical Engineering, Technische Univerität Darmstadt *Towards data-driven multi-scale modeling of soft, anisotropic lattice structures and meta-materials.*
12:15	**Lunch** (Mies-van-der-Rohe-Straße 10)	
13:30 - 13:55	Session 6	**Matthias Wieler**, F. Wankmüller, A. Weber, P.W. Hoffrogge, D. Schneider, B. Nestler, P. Haremski, A. Maruscyzk, P. Lupetin Corporate Sector Research and Advance Engineering, Robert Bosch GmbH *3D analysis of observed and simulated microstructure evolution in SOFC anodes.*
13:55 - 14:20		**Selina Neuhaus**, K. Srivastava, S. Scholl, S. Diebels Applied Mechanics, Saarland University, Saarbrücken *Comparison between an anisotropic yield function and a crystal plasticity model in modeling the mechanical behavior of single bicrystals.*
14:20 - 15:00	Final discussion	

6 Abstracts

In the following, all abstracts are listed. All abstracts are provided in the **order of appearance** according to the schedule (see Section 5, p. 8).

The session of the presentation is shown at the bottom of each page.

An FFT based micro mechanics solver for brittle fracture

F. Ernesti[1], M. Schneider[1], T. Böhlke[1]

[1]: Institute of Engineering Mechanics (ITM), Karlsruhe Institute of Technology (KIT), Germany; *mail:* {felix.ernesti, matti.schneider, thomas.boehlke}@kit.edu

The description of material failure as an energy minimization problem, i.e., the Francfort–Marigo model **[1]**, has been studied widely in recent years. The approximation of the crack surface as a phase field, i.e., smeared interface, enjoys great popularity, as it allows describing fracture as a set of partial differential equations.
In numerical homogenization, FFT-based solution methods have been established over the past two decades **[2]**. Their purpose is to compute the overall response of a heterogeneous microstruture wrt a macroscopic loading and can be applied to a variety of nonlinear materials. The balance of momentum is reformulated as a Lippmann-Schwinger fixed point equation and discretized on a regular voxel grid. The benefits lie in a fast implementation and the possibility to use image data like CT-scans as input without further need for meshing. The iterative solution methods do not require any linearization.
This talk presents the results of the masterthesis **[3]**. We investigate phase field crack propagation **[4]** on heterogeneous microstructures using FFT-based **[5]** solvers. We derive the Lippmann–Schwinger equations characterizing the critical points of the Ambrosio–Tortorelli functional. The equations are discretized by a trigonometric collocation method. In addition to the conventional alternating minimization algorithm we present accelerated methods.
With the introduced solver, we investigate the brittle behavior of different heterogeneous microstructures. Numerical tensile experiments with 2D spherical inclusions show the convergence behavior of the solver. A numerical investigation of the crack surface through a 3D fiber reinforced composite exhibits the advantages of the former introduced methods.

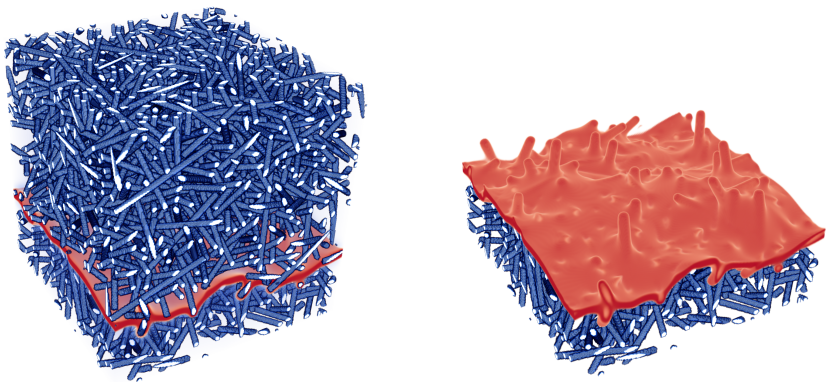


Figure 1: Crack path through a fiber reinforced composite

References

[1] G. A. Francfort and J.-J. Marigo [1998]. “Revisiting brittle fracture as an energy minimization problem“, Journal of Mechanics Physics of Solids **46**, 1319–1342

[2] H. Moulinec and P. Suquet [1998]. “A numerical method for computing the overall response of nonlinear composites with complex microstructure“, Computer Methods in Applied Mechanics and Engineering **157**, 69–94

[3] F. Ernesti [2018] “An FFT-based solver for brittle fracture on heterogeneous microstructures“, MSc thesis, Karlsruhe Institute of Technology (KIT), Institute of Engineering Mechanics

[4] B.Bourdin, G. A. Francfort and J.-J. Marigo [2000]. “Numerical experiments in revsited brittle fracture“, Journal of the Mechanics and Physics of Solids **48**, 797–826

[5] M. Schneider [2017] “An FFT-based fast gradient method for elastic and inelastic unit cell homogenization problems‘. Computer Methods in Applied Mechanics and Engineering **315**, 846–866

Computational homogenization of Sheet Molding Compound composites based on generated unit cells

J. Görthofer[1], M. Schneider[1], A. Hrymak[2], T. Böhlke[1]

[1]: Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Germany; *mail:* johannes.goerthofer@kit.edu, matti.schneider@kit.edu, thomas.boehlke@kit.edu

[2]: Department of Chemical and Biochemical Engineering, University of Western Ontario (UWO), Canada; *mail:* ahrymak@uwo.ca

Sheet Molding Compound (SMC) composites provide a good formability, low cycle times and a high function integration potential. SMC composites are manufactured via compression molding based on randomly distributed fibers within a pre-preg matrix, leading to a process dependent, heterogeneous structure. During the process, fibers tend to remain within their rovings and form a layered bundle structure. Therefore, SMC exhibits a three scale structure, namely fibers on the microscale, bundles on the mesoscale and unit cells on the macroscale. To apply SMC composites as structural components, their mechanical behavior needs to be understood and predicted precisely.

A glass-fiber SMC based on an unsaturated Polyester Polyurethane hybrid resin system (UPPH) is investigated **[1]**. To better understand the effective mechanical behavior of this SMC composite, the microstructure generator of Chen et al. **[2]** is extended and used as mutable input for fast Fourier transform (FFT) based full-field simulations **[3]**. Fig. 1 shows a generated bundle structure and the corresponding local stress field in x-direction due to a loading in x-direction, respectively.

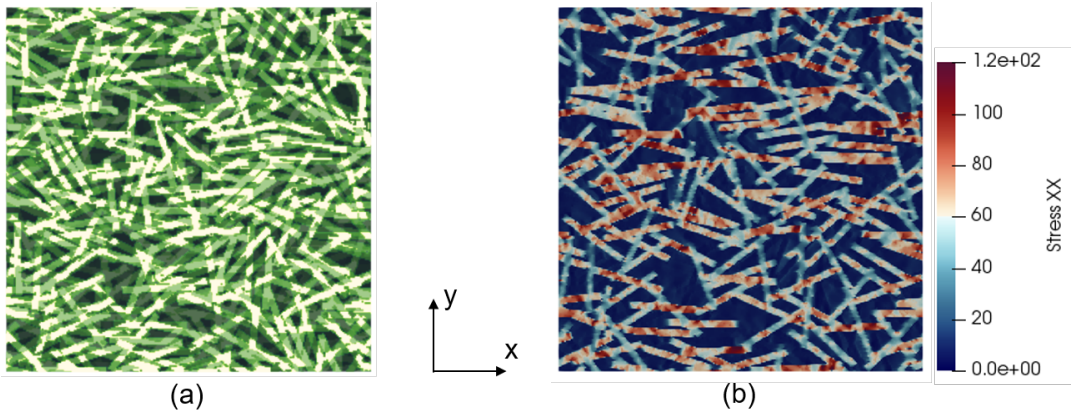


Figure 1: SMC composite mesostructure: (a) generated bundles in a unit cell, (b) computed stress in x-direction via FFT

References

[1] D. Bücheler, F. Henning [2016]: “Hybrid resin improves position and alignment of continuously reinforced prepreg during compression co-molding with Sheet Molding Compound”, 17th European Conference on Composite Materials, 6699–6703

[2] Z. Cheng, T. Huang, Y. Shao, Y. Li, H. Xu, K. Avery, D. Zeng, W, Chen, X. Su [2018]: “Multiscale finite element modeling of sheet molding compound (SMC) composite structure based on stochastic mesostructure reconstruction”, Composite Structures **188**, 25–38

[3] H. Moulinec, P. Suquet [1998]: “A numerical method for computing the overall response of nonlinear composites with complex microstructure”, Computational Methods in Applied Mechanics and Engineering **157**, 69–94

Homogenization for large deformations based on in silico data

O. Kunc[1,2], F. Fritzen[1]

[1]: Efficient Methods for Mechanical Analysis, University of Stuttgart
[2]: *mail:* kunc@mechbau.uni-stuttgart.de

We address the task of mechanical two-scale homogenization by means of dedicated interpolation methods. In principle, hyperelastic solids allow for an iteration-free description of the material behavior, e.g.

$$\mathbf{F} \mapsto \mathbf{P} = \frac{\partial W}{\partial \mathbf{F}}, \; \mathbb{C} = \frac{\partial^2 W}{\partial \mathbf{F} \partial \mathbf{F}}$$

with the deformation gradient $\mathbf{F}$, the stored energy function W, the first Piola-Kirchhoff stress tensor $\mathbf{P}$, and the corresponding tangent modulus.

Since these relationships are conserved under the transition to the macro-scale, it is self-evident that, in principle, one could overcome the burden of solving the microscopic boundary value problem at all.

This method is an extension of the RNEXP method from **[1]** to the regime of finite strains. It is based on efficient sampling of the deformation gradient's isochoric part $\widetilde{\mathbf{F}} = J^{-1/3}\mathbf{F}$ and a separate treatment of it's volumetric contribution $J = \det \mathbf{F}$.

The data necessary for the interpolation is provided by a reduced order model, which itself is based on the same sampling strategy.

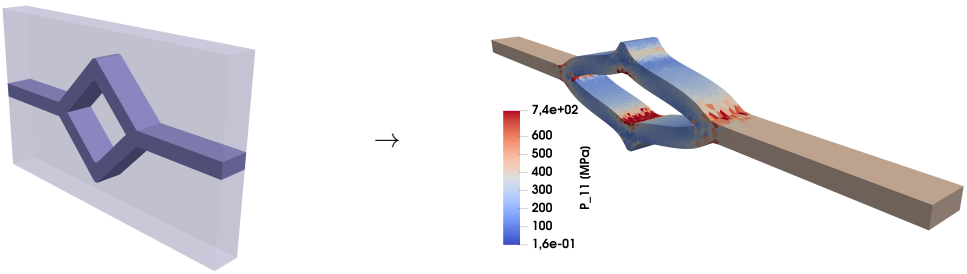


Figure 1: Example of a deformation with pronounced geometric nonlinearity.

Fig. **2** exemplifies a scenario when geometric nonlinearities are of high importance. The corresponding stiffening effect is accurately reproduced by our method. First realistic two-scale simulations are anticipated.

References

[1] F. Fritzen, O. Kunc [2018]: "Two-stage data-driven homogenization for nonlinear solids using a reduced order model", European Journal of Mechanics / A Solids **69**, 201–220

Machine learning and data mining applications for identification of key dependencies across multiple scales in continuum materials mechanics

F. Bock[1], R. Aydin[1], C. Cyron[1,2], N. Huber[1,3], S. Kalidindi[4], B. Klusemann[5]

[1]: Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany; *mail:* frederic.bock@hzg.de

[2]: Institute of Continuum and Materials Mechanics, Hamburg University of Technology (TUHH), Hamburg, Germany

[3]: Institute of Materials Physics and Technology, Hamburg University of Technology (TUHH), Hamburg, Germany

[4]: School of Mechanical Engineering and School of Computational Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States of America

[5]: Institute of Product and Process Innovation, Leuphana University of Lüneburg, Lüneburg, Germany

For enabling accelerated development of novel materials that are most suitable for their designated purpose, data analytical methods, in particular machine learning approaches, represent powerful tools. The identification of key dependencies along the process-microstructure-property-performance (p-s-p-p) chain of materials often requires the coupling of multiple spatiotemporal scales involving multiphysics. An overview of different common data structures of sources relevant for data analytics within continuum materials mechanics is provided in Fig. 2. The particular machine learning approach most appropriate for any use-case highly depends on involved data types, formats, spatiotemporal scales, affordable computational costs as well as existing knowledge to be transferred and anticipated understanding to be gained.

For our purposes, machine learning tasks broadly fall into at least one of these categories: descriptive, predictive and prescriptive. Descriptive tasks, for example, include methods such as pattern recognition and correlation, predictive tasks can involve classification or statistical inference and predictive tasks are performed for implementing proposed optimization. Various variants of artificial neural networks, support vector machines and random forests as well as Bayesian inference and principal component analysis can be utilized for these tasks. With these methods, challenges that involve connecting process parameters to microstructural classification and feature extraction as well as to mechanical properties and fatigue performance behaviour can be faced. In this contribution, examples of machine learning methods for the identification of relationships along the p-s-p-p chain will be reviewed.

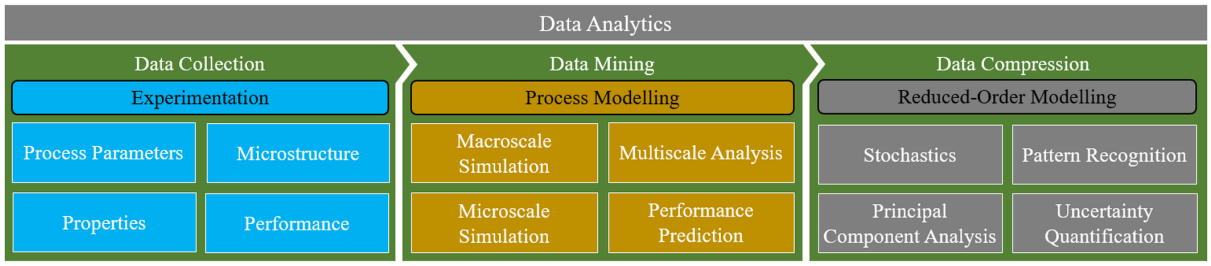


Figure 1: Overview of different data sources and data processes relevant for data analytics within the field of continuum materials mechanics. Own image based on the idea presented by **[1]**.

References

[1] J. Smith et al. [2016]: “Linking process, structure, property, and performance for metal-based additive manufacturing: Computational approaches with experimental support”, Computational Mechanics **57** 583 - 610.

Data-driven stress prediction for failure analysis

K. Schulz[1], S. Kreis[1], N. Magino[1], H. Trittenbach[2]

[1]: Institute of Applied Materials (IAM-CMS), Karlsruhe Institute of Technology, Germany; *mail:* katrin.schulz@kit.edu
[2]: Institute of Program Structures and Data Organization, Karlsruhe Institute of Technology, Germany.

Advanced data analysis is increasingly popular with materials engineering. There are many interesting applications, e.g., to identify links between material properties and structural behavior. Most of these applications also entail challenges like compliance with safety requirements for parts and components. These challenges often are specific to the engineering domain, which sets them apart from many other disciplines where data-science already is established. To successfully approach materials science problems with machine learning, one has to identify and address these specifics **[1]**.

In this contribution, we pursue this question for the investigation of internal stress states in the context of failure analysis. More specific, we first study whether the prediction of critical stress states is feasible only based on surface measurements of a three-point bending structure. To this end, we pursue several approaches to gain insights into crack initiation and material behavior. We compare different data sets and machine-learning methods to identify variables, such as specific surface locations, that are relevant for high prediction accuracy. Based on our analyses, we discuss the applicability and general principles of machine learning for materials engineering. Finally, we extend the investigation to microscale considerations of plastic deformation. We analyze discrete dislocation systems in order to find adequate homogenization approaches to capture relevant mechanisms of microstructural evolution for continuum plasticity models. The heterogeneity of internal stress states due to plastic evolution on different slip systems is exemplarily shown in Fig. **2**.

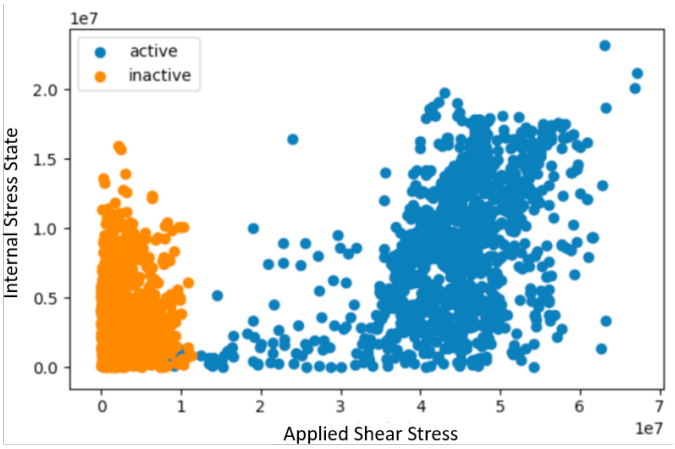


Figure 1: Voxel-based stress evaluation of microstructure evolution of a tension test.

References

[1] Trittenbach, H., Gauch, M., Böhm, K., Schulz, K. [2018]: “Towards Simulation Data Science - A Case Study on Material Failures”. Proceeding of 5th International Conference on Data Science and Advanced Analytics (DSAA), pp. 450-459, IEEE.

Usage of data to create efficient surrogate models and to train low-rank approximations

S. Kastian[1], S. Reese[1]

[1]: Institute of Applied Mechanics, RWTH University Aachen, Germany; *mail:* {steffen.kastian, stefanie.reese}@rwth-aachen.de

In many cases a large amount of data is generated (e.g. experiments or numerical simulations). These data can be used advantageously in various ways. Be it as a replacement for the constitutive law, investigation of a certain quantity of interest (qoi) or for generating surrogate models. However, the possibility must be considered that certain data can be disadvantageous for the respective area of application. This may be caused by incorrect or irrelevant data.

The new adaptive proper orthogonal decomposition (APOD) **[1]** method is introduced in this contribution to create surrogate models of certain simulations. Based on the proper orthogonal decomposition (POD) **[2]**, both, POD and APOD requires a certain database to create projection matrices. The same database is used for both methods, but the APOD takes adaptively a certain selection of data into account and thus neglects the data that are not relevant for the current situation. This can improve either accuracy or speed.

Many engineering relevant problems can be attributed to a certain number of quanitity of interest. If data already exist for the problem under investigation, they can be used to train low rank approximation, which can approximate the qoi for non-existent data. These data can also be generated from previously mentioned surrogate models. Therefore, the hierarchical tensor approximation (HTA) **[3]** is combined with (A)POD to generate required training data efficiently. Further the results of HTA are compared with the results of the full model.

References

[1] S. Kastian, S. Reese [2018]: “An adaptive way of choosing significant snapshots for the Proper Orthogonal Decomposition“, IUTAM bookseries, accepted (December 03, 2018)

[2] A. Radermacher, S. Reese [2013]: “Proper orthogonal decomposition-based model reduction for nonlinear biomechanical analysis“, International Journal of Materials Engineering Innovation, Special Issue on Computational Mechanics and Methods in Applied Materials Engineering;

[3] D. Pivovarov, K. Willner, P. Steinmann, S. Brumme, M. Müller, T. Srisupattarawanit, G.-P. Ostermeyer, C. Henning, T. Ricken, S. Kastian, S. Reese, D. Moser, L. Grasedyck, J. Biehler, M. Pfaller, W. Wall, T. Kolsche, O. v. Estorff, R. Gruhlke, M. Eigel, M. Ehre, I. Papaioannou, D. Straub, S. Leyendecker [2019]: “Challenges of order reduction techniques for problems involving polymorphic uncertainty“, GAMM Mitteilungen, accepted (January 24, 2019)

Artificial neural networks for the modeling of the constitutive behavior of materials

S. Freitag[1]

[1]: Institute for Structural Mechanics, Ruhr University Bochum, Germany; *mail:* steffen.freitag@sd.rub.de

Artificial neural networks are powerful tools to identify dependencies between input and output data in the framework of data-driven modeling. They can be trained with data obtained from experiments (measurements of lab experiments or in situ monitoring) or with results of numerical simulations, i.e. as surrogate models to replace time consuming simulation models. Some applications of artificial neural networks in structural mechanics are presented in **[1]**. This contribution is focused on artificial neural networks for the modeling of stress-strain-dependencies to be applied as constitutive material models within structural simulations, e.g. by means of the finite element method, see e.g. **[2]**. Special network architectures for anisotropic, orthotropic and isotropic material behavior are discussed. Exemplified in Fig. **2**, a sub structured artificial neural network with symmetric synaptic connections is shown, which can be used for the modeling of isotropic elastic material behavior. It should be noted, that at least six hidden neurons are required, but the number of hidden neurons can be increased to capture more complicated material nonlinearities. The modeling of time dependent behavior (e.g. viscoelasticity) can be solved with recurrent neural networks **[3]**. In **[4]**, a recurrent neural network is trained to approximate fractional rheological models, which require to take the whole strain history into account to predict the current stress state.

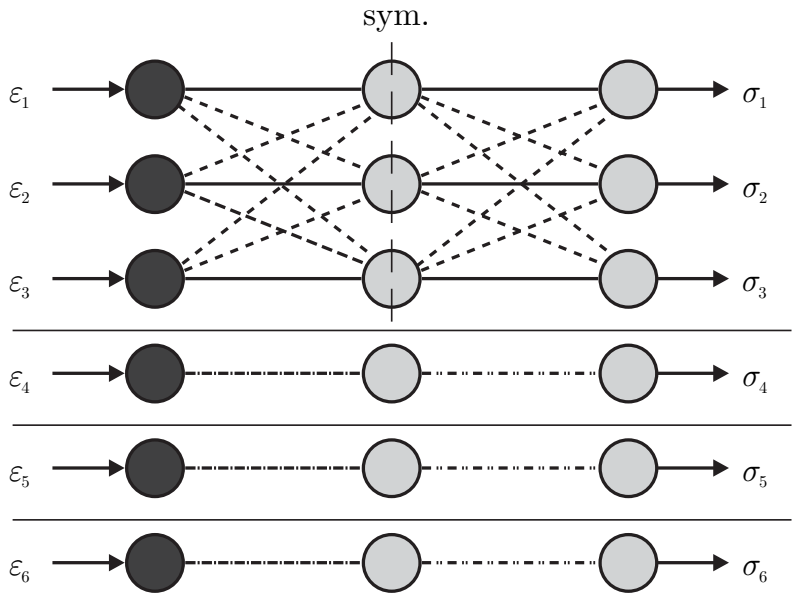


Figure 1: Artificial neural network with feed forward architecture for isotropic elastic material behavior

References

[1] S. Freitag [2015]: “Artificial Neural Networks in Structural Mechanics”, In: Y. Tsompanakis, J. Kruis, B.H.V. Topping (eds.), Computational Technology Reviews, Saxe-Coburg Publications, Stirlingshire, Volume 12, pp. 1–26

[2] Y.M.A. Hashash, S. Jung, J. Ghaboussi [2004]: “Numerical implementation of a neural network based material model in finite element analysis”, International Journal for Numerical Methods in Engineering **59**, 989–1005

[3] S. Freitag, W. Graf, M. Kaliske [2013]: “A material description based on recurrent neural networks for fuzzy data and its application within the finite element method”, Computers & Structures **124**, 29–37

[4] M. Oeser, S. Freitag [2016]: “Fractional derivatives and recurrent neural networks in rheological modelling – part I: theory”, International Journal of Pavement Engineering **17**, 87–102

Deep learned (micromechanical) constitutive modeling of hyperelastic materials

K. Linka[1], M. Hillgärtner[2], C. Cyron[1]

[1]: Department of Continuum and Materials Mechanics, Hamburg University of Technology, Germany; *mail:* kevin.linka@tuhh.de
[2]: Department of Continuum Mechanics, RWTH Aachen University, Germany

Modern material measurement techniques have developed rapidly over the last decades and evolved from purely one-dimensional macroscopic to multi-dimensional techniques manageable of linking the microstructural kinematics to macroscopical material responses. Accordingly, the opportunities of advanced data-driven modeling strategies increased as well as the chances to tune the material behavior towards its optimum for a particular boundary-value problem. To this end, we propose a modeling approach based on the principles of invariant hyperelasticity in conjunction with micromechnical material information incorporated into a feedforward fully connected artificial neural network (ANN). Moreover, the ANN architecture was specifically designed to be robust against the chosen hyperparameters, while still being numerically efficient. We evaluate the predictive capabilities of trained ANNs against analytical and numerical examples. In addition, a computational homogenization analysis of an representative volume element by varying the micromechanical properties and comparing the macroscopic stress responses against the ones learned by ANNs, was performed. Hence, the present study provides considerable insights for the possibility of a material data-driven methodology of developing constitutive laws based on measured material information.

Towards deep learned constitutive models based on two-dimensional strain fields

M. Hillgärtner[1], K. Linka[2], M. Itskov[1]

[1]: Department of Continuum Mechanics, RWTH Aachen University, Germany; *mail:* hillgaertner@km.rwth-aachen.de

[2]: Institute of Continuum and Materials Mechanics, Hamburg University of Technology, Germany

In order to calibrate material models, experimental stress-strain curves are usually compared with model predictions under the same loading conditions. While this approach guarantees good results for one specific loading type, the resulting model is not generally able to properly predict other loading scenarios. Therefore, a variety of mechanical tests can be conducted, amongst which uniaxial tension, uniaxial compression, pure-shear and equibiaxial tension tests are the most commonly used ones. Multi-axial loading often cannot be adequately predicted solely based on test data of one such idealized test. Therefore, the material model can be fitted against several mechanical test data sets simultaneously in order to increase the prediction quality, which requires a considerable amount of experiment work.

This contribution aims to create phenomenological material models which are directly fitted against an experimental force response and the corresponding two-dimensional strain field obtained from arbitrary loading. To this end, a deep learning framework based on a multilayer-perceptron (MLP) approach **[1]** is proposed which identifies suitable strain-energy functions and its corresponding derivatives. These can be utilized in a commercial finite element code via a user defined material subroutine in order to compare the quality of the approximation with the reference data. This approach skips idealized experiments and simplifies the process of phenomenological modeling by exploiting the capabilities of deep neural networks.

References

[1] I. Goodfellow, Y. Bengio, A. Courville [2016]: ”Deep Learning”, MIT Press.

A general approach for model-free data-driven inelasticity

R. Eggersmann[1], T. Kirchdoerfer[2], S. Reese[1], L. Stainier[3], M.Ortiz[2,4]

[1]: Institute of Applied Mechanics, RWTH Aachen University, Mies-van-der-Rohe-Str. 1, D-52074 Aachen, Germany; *mail:* robert.eggersmann@ifam.rwth-aachen.de
[2]: Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 91125, USA; *mail:* ortiz@aero.caltech.edu
[3]: Institute of Civil and Mechanical Engineering, École Centrale de Nantes, 1 Rue de la Noë, F-44321 Nantes, France; *mail:* Laurent.Stainier@ec-nantes.fr
[4]: Hausdorff Center for Mathematics, Universität Bonn, Endenicher Allee 60, 53115 Bonn, Germany

To motivate a data-driven reformulation of the initial boundary value problem, we just have to consider that the world we live in today is a data-rich one. Measurement techniques are improving as well as the amount of data we can deal with. We extend the data-driven formulation introduced by Kirchdoerfer and Ortiz [1] to any kind of inelastic material behavior in theory [2]. We make use of the fact, that material behavior can always be described by its entire deformation history $\boldsymbol{\sigma}(t) = \hat{\boldsymbol{\sigma}}(\{\boldsymbol{\varepsilon}(s)\}_{s\leq t})$, where $\boldsymbol{\sigma}(t)$ is the stress at time t and $\hat{\sigma}(\bullet)$ is a general function of the whole deformation history. Besides, the effect of fading memory properties gives more power to this formulation. Where fading memory properties mean that for many materials the shorter history of deformation is of higher importance to the actual material behavior. To include this theoretical procedure into the data-driven algorithm, we adapt the double minimum problem by history-matching

$$\min_{\boldsymbol{z}_{k+1}\in E_{k+1}} \min_{\{\boldsymbol{y}_k,\boldsymbol{y}_{k+1}\}\in H} d\big(\{\boldsymbol{y}_k,\boldsymbol{y}_{k+1}\},\{\boldsymbol{z}_k,\boldsymbol{z}_{k+1}\}\big). \tag{1}$$

Here, $\boldsymbol{y}_{k+1}$ and $\boldsymbol{z}_{k+1}$ are pairs of stress and strain at a discretized time step $k+1$, E_{k+1} is the according constraint set, H the history data set and d a distance measure. The formulation above shows the history-matching formulation for materials with short memories. Already this simple formulation is able to deal with several material effects which are of a first order differential relation, like certain types of visco-elasticity, ideal visco-plasticity, or plasticity with kinematic hardening.

To verify the above formulation, we performed several computations at truss structures, where each truss can only be loaded in the normal direction (1D problem). The problem shows convergence with an increasing number of data points towards the reference solution. Multi-dimensional problems will also be discussed in the presentation.

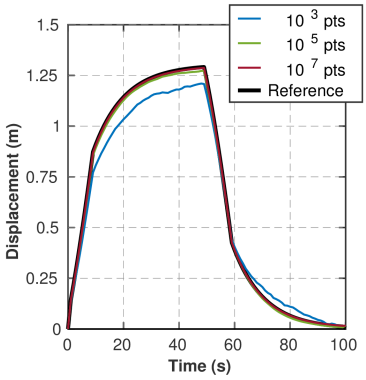


Figure 1: Visco-elastic problem for loading 10 sec. and unloading after 50 sec. again within 10 sec. Convergence towards a displacement response at a certain node with an increasing number of data points.

References

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

[2] Eggersmann R., Kirchdoerfer T., Reese S., Stanier L., Ortiz M. [2018], Model-free data-driven inelasticity, ArXiv e-prints, arXiv:1808.10859.

Data-driven finite strain elasticity

A. Platzer[1], M. Ortiz[2], L. Stainier[1], A. Leygue[1]

[1]: Institut de Recherche en Génie Civil et Mécanique (GeM - UMR 6183 CNRS/ECN/UN), Ecole Centrale Nantes, F-44321 Nantes, France; *mail:* auriane.platzer@ec-nantes.fr
[2]: Graduate Aerospace Laboratories, California Institute of Technology, Pasadena, CA 91125, USA; *mail:* ortiz@aero.caltech.edu

The unknowns of a boundary value problem (BVP) in mechanical engineering are (i) the displacement field, (ii) the strain field, and (iii) the stress field. The corresponding governing equations are of two types: first, both equilibrium and compatibility equations, which derive from universal laws; second, mechanical constitutive equations, generally subject to various modeling assumptions, which inevitably introduces a bias in the solution. To overcome this issue, Kirchdoerfer and Ortiz (2016) proposed a new paradigm, called *data-driven computational mechanics*, which consists in substituting the constitutive model with a database of strain-stress couples **[1]**. They demonstrate the relevance of this approach with linear elastic manufactured data.

Nguyen and Keip (2018) proposed an extension of this framework to large strain elasticity **[2]**. In their work, the material database is constituted of Green-Lagrange strain - second Piola-Kirchhoff stress couples, referred to as *material states*. The solution of the BVP is a set of *mechanical states*, which collects strain-stress couples both (i) verifying universal laws and (ii) closest to the material dataset. Practically, the resolution consists in minimizing the distance between the mechanical state of all material points in the body and the material database, under equilibrium and compatibility constraints. In the Lagrangian framework, the non-linearity of these constraints yields a nonlinear and coupled system for the displacements and the Lagrangian multipliers enforcing equilibrium **[2]**. The impact of this non-linearity and the question of convergence with respect to dataset has not yet been explored.

We therefore here propose to formulate data-driven finite strain elasticity in the phase-space of the deformation gradient - first Piola-Kirchhoff stress tensor: the compatibility and equilibrium, and thus the optimization constraints, are now linear functions of the displacements. The method is assessed on 2D elastic finite strain problems. As a discussion, the results are compared to the Lagrangian approach, modified with some enhancements to the original algorithm. Together with the influence of some parameters of the algorithm, the robustness of the method with regard to the richness of the database is also investigated.

References

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

[2] L.T. Nguyen, M.A. Keip [2018]: “A data-driven approach to nonlinear elasticity". Computers and Structures, **194** 97–115

Towards data driven finite element analysis

T. Korzeniowski[1], K. Weinberg[1]

[1]Institute of Solid Mechanics, University of Siegen, Germany; *mail:* tim.korzeniowski@uni-siegen.de

The data driven finite element formulation of Kirchdoerfer and Ortiz **[1]** is a promising approach to reduce uncertainties in the material modeling step. In the data driven finite element analysis the constitutive material modeling is eluded and instead experimental data are directly employed as an input for computational analysis. Our contribution discusses the implementation of material uncertainties by this method. We therefore compare this approach to more traditional finite element methods. The point of departure is a given set of noisy material data which requires simplification and / or uncertainty modeling of the material. We illustrate the methodology of data driven solutions, stochastic finite element solutions and analytic solutions under such material uncertainties. Numerical examples are used to show the pros and cons of the given methods. Furthermore we explore the usage of the data driven modeling within different applications and also take a look on the acquisition of the multi-dimensional data fields needed. Furthermore the data driven problem is expressed by a distance minimizing problem; we search for the data point which is closest to satisfying the conservation laws. To reduce computational cost in this search we introduce a multi-level data set approach to encounter this problem. We provide several examples where we investigated the behavior of the data driven approach with respect to the previously named problems.

References

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

[2] T. Korzeniowski, K. Weinberg [2019]: “A stochastic and a data driven FEM approach to problems with insufficient material data.”, Computer Methods in Applied Mechanics and Engineering, subm.

Model-Free Data-Driven Computing

M. Ortiz[1,2]

[1]: Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 91125, USA; *mail:* ortiz@aero.caltech.edu
[2]: Hausdorff Center for Mathematics, Universität Bonn, Endlicher Allee 60, 53115 Bonn, Germany

We develop a new computing paradigm, which we refer to as Data-Driven Computing, according to which calculations are carried out directly from experimental material data and pertinent kinematic constraints and conservation laws, such as compatibility and equilibrium, thus bypassing the empirical material modeling step of conventional computing altogether. Data-driven solvers seek to assign to each material point the state from a prespecified data set that is closest to satisfying the conservation laws. Equivalently, data-driven solvers aim to find the state satisfying the conservation laws that is closest to the data set. The resulting data-driven problem thus consists of the minimization of a distance function to the data set in phase space subject to constraints introduced by the conservation laws. We demonstrate the data-driven paradigm and investigate the performance of data-driven solvers by means of several examples of application, including statics and dynamics of nonlinear three-dimensional trusses, and linear and nonlinear elasticity. In these tests, the data-driven solvers exhibit good convergence properties both with respect to the number of data points and with regard to local data assignment, including noisy material data sets containing outliers. The variational structure of the data-driven problem also renders it amenable to analysis. We find that the classical solutions are recovered in the case of linear elasticity. We identify conditions for convergence of Data-Driven solutions corresponding to sequences of approximating material data sets. Specialization to constant material data set sequences in turn establishes an appropriate notion of relaxation. We find that relaxation within the Data-Driven framework is fundamentally different from the classical relaxation of energy functions. For instance, we show that in the Data-Driven framework the relaxation of a bistable material leads to effective material data sets that are not graphs. I will finish my presentation with highlights on work in progress, including closed-loop Data-Driven analysis and experiments, Data-Driven molecular dynamics, Data-Driven inelasticity and publicly-editable material data repositories and data management from a Data-Driven perspective.

Artificial Neural Networks as Surrogate Models

A. Mielke[1], T. Ricken[2]

[1]: Institute of Mechanics, Structural Analysis, and Dynamics, University of Stuttgart; *mail:* andre.mielke@isd.uni-stuttgart.de

[2]: Institute of Mechanics, Structural Analysis, and Dynamics, University of Stuttgart; *mail:* tim.ricken@isd.uni-stuttgart.de

Machine learning techniques have found many applications in various fields. Their role in the mechanics community is still subject to ongoing debate and research. Of these techniques artificial neural networks (ANN) gained a lot of traction in recent years thanks to overwhelming and unexpected success in practical as well as previously thought unsolvable problems **[1]**.
One use case for ANN is to create surrogate models for differential equations. Instead of time-consuming full simulations, approximations can be made with in principal arbitrarily small error, given the solution of the differential equation is continuous **[2]**. Such a network would be trained by simulation data spanning the whole solution space.
We trained a simple ANN as a surrogate for a nonlinear coupled biomechanical model of a liver lobule **[3]** using the final fat volume fraction n^T as the output parameter. As an error quantifier, we averaged the relative approximation error on the test set for each node and derived the cumulative error for the whole system as the average and standard deviation of the averaged errors (cf. Fig. 1). To improve results, more complex network topologies and hyperparameter tweaking have to be employed alongside gaining more data.
Open questions are the possibility of using adaptive sampling techniques to reduce bias towards lumped solution data (cf. Fig. 2) and a priori error estimates for approximating unknown functions.

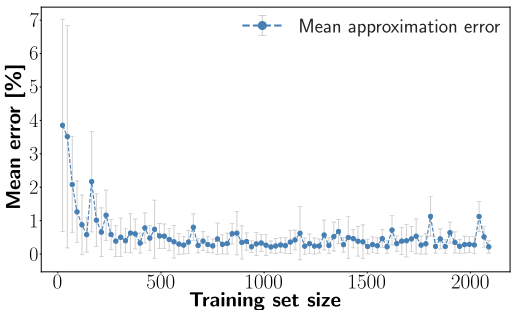


Figure 1: Cumulative approximation error for a simple surrogate ANN model on a PDE-ODE model of a liver lobule

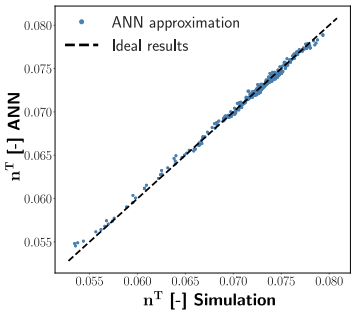


Figure 2: ANN approximated fat volume fraction vs. simulation result exemplarily plotted for node 15 to show lumping towards overrepresented solutions in the data set

References

[1] D. Silver et al. [2016]: “Mastering the Game of Go with Deep Neural Networks and Tree Search”, *Nature* **529**, 484–489

[2] V. Kreinovich [1990]]: “Arbitrary Nonlinearity is Sufficient to Represent All Functions by Neural Networks: A Theorem”, *Neural Networks* 4 **3**, 381–383

[3] T. Ricken et al. [2015]]: “Modeling Function-Perfusion Behaviour in Liver Lobules Including Tissue, Blood, Glucose, Lactate and Glycogen by Use of a Coupled Two-scale PDE-ODE Approach”, *Biomechanics and modeling in mechanobiology* **14.3**, 515–536

Data-Driven Microstructure Property Relations

J. Lißner[1], F. Fritzen[1]

[1]: Institute of Applied Mechanics, University of Stuttgart, Germany; *mail:* {lissner,fritzen}@mechbau.uni-stuttgart.de

Effective material properties of highly heterogeneous materials are induced by their microscale, being defined on a length scale of around 10^{-6} relative to the macroscopic domain size **[1]**. The concept of the representative volume element (RVE), which describes the microscale with one representative frame, is usually deployed. Nevertheless, computations on this frame are still quite costly and an efficient method to accurately predict the material property is sought-after.
The microstructures deployed in this study are randomly generated. Each generated RVE is influenced by various parameters, the phase volume fraction of the inclusions, the shape and size of the inclusions, as well as the overlap of the inclusions. The randomly assigned overlap allows for a model of soft and hard inclusions in each RVE. The goal is an image based prediction for the heat conductivity, i.e. a method that gets away without micsrostructural parameters such as the number and shape of inclusions etc.
Using machine learning **[2]**, patterns and characteristic properties of the RVEs are identified during unsupervised learning. The outcome of the unsupervised learning is the definition of a feature vector that is used for the subsequent supervised learning. During feature identification we make use of the two point spatial correlation function which describes a probability distribution of the RVE, which is governed by randomness. This property of the two point spatial correlation function is exploited with a snapshot proper orthogonal decomposition (POD) which is deployed in order to identify patterns within the various snapshots. With the sheer number of snapshots required to compute a salient reduced basis (RB) adequately representing the parameter range, the necessity for an incremental scheme arises. Three different methods are introduced for the incremental computation of the RB. After training of the RB, it is used to extract salient features of the RVE written into the feature vector.
With the feature vector at hand, an artificial neural network (ANN) is deployed as a regression model. Therefore, a dense feed forward ANN is trained to predict the heat conductivity for the given feature vector, which is obtainable with just the image of the RVE.

References

[1] Torquato, S. [2013]: ”Random heterogeneous materials: microstructure and macroscopic properties”; Vol. 16, Springer Science & Business Media, 2013.

[2] Nasrabadi, N.M. [2007]: ”Pattern recognition and machine learning”, Journal of electronic imaging **2007**,16,049901.

Towards data-driven multi-scale modeling of soft, anisotropic lattice structures and metamaterials

O. Weeger[1,2]

[1]: Cyber-Physical Simulation Group, Department of Mechanical Engineering, Technische Universität Darmstadt, Germany; *email:* weeger@cps.tu-darmstadt.de

[2]: SUTD Digital Design and Manufacturing Centre, Singapore University of Technology and Design, Singapore;

Additive manufacturing now enables the fabrication of architectured cellular materials such as soft, functionalized, multi-material lattice structures and heterogeneous metamaterials. This provides completely new dimensions of design freedom to be explored, such as large-deformations, instabilities, functional grading, anisotropy, and multi-functional behavior. To maintain precise control of structural behavior through tailoring of micro-structural design and process parameters, efficient multi-scale modeling and simulation methods are essential. However, multi-scale simulation is particularly challenging for functional structures that are characterized by large deformations, anisotropy, nonlinear, inelastic, and multi-functional material behavior, since homogenized constitutive properties of the micro-structure and their dependence on design parameters need to be captured and represented for sequential approaches.

Based on our previous work on full-scale simulation of nonlinear, conformal and graded lattice structures **[1]**, see Fig. 1, we are developing a multi-scale simulation and design framework for nonlinear lattice structures and metamaterials. Particular challenges to be addressed include nonlinearity (stemming from large deformation of the microstructure), anisotropy (grading of lattice struts) and non-periodicity (due to conformity of macroscopic geometry and morphing of unit cells). Thus, we want to explore the use of data-driven and machine learning methods for computational homogenization and reduced-order or surrogate modeling of the microscopic constitutive behavior **[2]**,**[3]**.

The objective of this talk is to introduce the general topic and idea, present the current progress, and discuss challenges faced and to be adressed in future research.

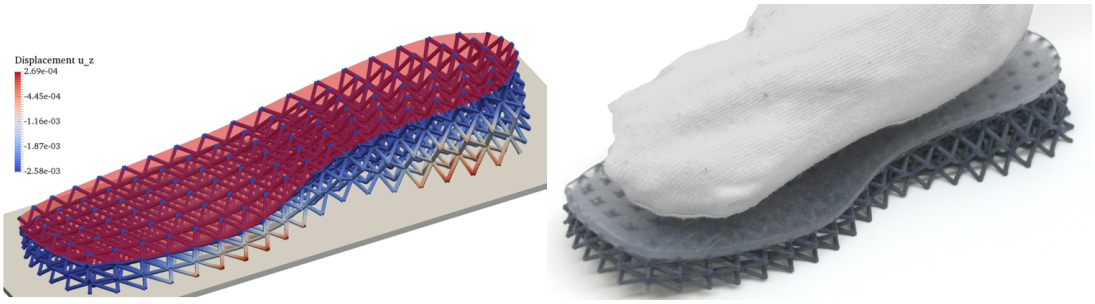


Figure 1: Full-scale simulation and 3D printing of a *soft* lattice structure **[1]**

References

[1] O. Weeger, N. Boddeti, S.-K. Yeung, S. Kaijima, M.L. Dunn [2018]: “Digital Design and Nonlinear Simulation for Additive Manufacturing of Soft Lattice Structures”, Addit. Manuf. **25**, 39–49

[2] J. Yvonnet, E. Monteiro, Q.-C. He [2013]: “Computational Homogenization Method and Reduced Database Model for Hyperelastic Hetereogeneous Structures”, Int. J. Multiscale Comput. Eng. **11**(3)

[3] B.A. Le, J. Yvonnet, Q.-C. He [2015]: “Computational homogenization of nonlinear elastic materials using neural networks”, Int. J. Numer. Methods Eng. **104**(12), 1061–1084

3D analysis of observed and simulated microstructure evolution in SOFC anodes

M. Wieler[1], F. Wankmüller[2], A. Weber[2], P.W. Hoffrogge[3], D. Schneider[3], B. Nestler[3], P. Haremski[1,3], A. Marusczyk[1], P. Lupetin[1]

[1]: Corporate Sector Research and Advance Engineering, Robert Bosch GmbH, Robert-Bosch-Campus 1, 71272 Renningen, Germany; *mail:* matthias.wieler@de.bosch.com
[2]: Institute of Applied Materials, Karlsruhe Institute of Technology, Kaiserstrasse 12, 76131 Karlsruhe, Germany
[3]: Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Sciences, Moltkestrasse 30, 76133 Karlsruhe, Germany

Many functional composite materials have a complex microstructure that is crucial for the material's performance. We investigate porous composites of nickel and YSZ (yttria stabilized zirconia) that are used as anodes in full-ceramic solid oxide fuel cells (SOFC) **[1]**. An important degradation mechanism of SOFC anodes is the diffusional transport of nickel under operating conditions (post-sintering). The resulting microstructural changes have been analyzed with 3D FIB-SEM reconstructions, and simulated with large-scale multi-phase field simulations.

We present the results of 3D analyses of several data sets from FIB-SEM reconstructions and from phase field simulations. We calculate standard microstructural features of SOFC anodes such as volume fractions, active and inactive three-phase-boundary (3PB) length, and tortuosity, which we use to predict the performance of these anodes based on the transmission line model.

The main factor of degradation is loss of connectivity of the nickel phase. To investigate this, we carry out a bottleneck analysis to quantify the gradual tightening of the nickel bottlenecks. In addition, we calculate several shape descriptors such as interface areas and local structure size, which confirms quantitatively that nickel relocates from small pores to larger pores within the YSZ skeleton.

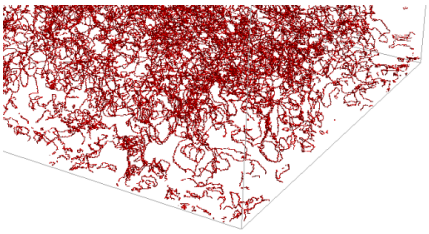


Figure 1: Distribution of triple phase boundaries

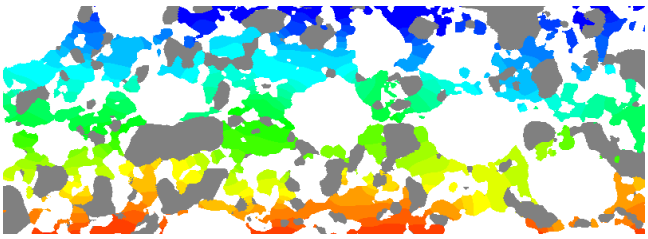


Figure 2: Electrical potential for calculation of tortuosity

References

[1] J.-C. Njodzefon, N. Maier, J. Schmieg, M. Meffert, H. Störmer, D. Gerthsen, P. Lupetin [2018]: "Performance and stability evaluation of a novel full-ceramic inert substrate-supported solid oxide fuel cell", Proc. 13th European SOFC & SOE Forum 2018

Comparison between an anisotropic yield function and a crystal plasticity model in modeling the mechanical behavior of single and bicrystals

S. Neuhaus[1], K. Srivastava[2], S. Scholl[2], S. Diebels[1]

[1]: Applied Mechanics, Saarland University, Saarbrücken; *mail:* selina.neuhaus@uni-saarland.de
[2]: AG der Dillinger Hüttenwerke, Dillingen

The microstructure of dual- and complex-phase steels, which is formed during the production processes of the metal plate, highly influences the mechanical properties. The preferred crystallographic orientations in the polycrystalline aggregate of the rolling textures causes an elastic-plastic anisotropy in these materials. The aim of the present work is to integrate plastic anisotropy in an already existing microstructure based model for the elasto-plastic deformation of dual-phase steels and thereby to widen the scope of such a model to a broader range of rolled steels.
The following contribution discusses the results of simulations on single- and bicrystals in the commercial finite element software ABAQUS® by using two different approaches, namely the Hill model **[1]** as a phenomenological yield function and a crystal plasticity model, to describe the anisotropic plastic behavior. The Hill model **[1]** is already implemented in ABAQUS® and was used to accomplish a deeper understanding of the behavior and applicability of an analytical, anisotropic yield function in describing anisotropically deforming metals. The simulation results with this model were compared to the results of simulations with the user-material subroutine of Huang **[2]** for a single crystal plasticity model, which was modified by Kysar **[3]**.

References

[1] R. Hill [1948]: “A theory of the yielding and plastic flow of anisotropic metals”, Proceedings of the Royal Society A, 193. Jg., Nr. 1033, 281–297.

[2] Y. Huang, [1991]: “A user-material subroutine incorporating single crystal plasticity in the ABAQUS finite element program, Mech Report 178”, Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts

[3] J. W. Kysar [1997]: “Addendum to ’A user-material subroutine incorporating single crystal plasticity in the ABAQUS finite element program, Mech Report 178”, Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts