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Helmholtz-Zentrum hereon

7th GAMM AG Data Workshop

December 15, 2021

Final Program

Online (ZOOM)

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 time, X-ray computed tomography devices are now available in many research facilities. By virtue of the obtained three-dimensional images, microstructures 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 within the GAMM AG Data. Innovative image processing techniques for automatic phase segmentation and microstructure reconstructions are of equal importance.

Objectives of the Workshop

- To discuss the state of the art and recent trends in data-driven approaches
- Extensive online poster sessions, allowing detailed discussions and exchanges

Topics of the workshop

- data-supported modeling of the constitutive behavior of materials
- data-driven simulation techniques
- machine learning tools for materials engineering
- high-performance data-processing
- microstructure generation, simulation and analysis, e.g. via machine learning or AI tools

Program

Wednesday, 15.12.2021
(https://leuphana.zoom.us/j/97181055405?pwd=b21wbVV5MVpjSUhjN0lCa3hnNlFzUT09)

13:10-13:25 **Opening / Welcome**

13:25-13:40 C. Tsegouog, P. Sharma, V. Dörlich, J. Linn, S. Diebels
New Experimental Characterisation of Cable Systems
Institute of Engineering Mechanics, Saarland University

13:40-13:55 J. Lißner, F. Fritzen
Convolutional Neural Networks - how to make them work for periodic image Data
Data Analytics in Engineering, University of Stuttgart

13:55-14:10 F.E. Bock, S. Keller, N. Huber, B. Klusemann
Hybrid modelling: Combining physics-based and data-driven modelling by enhancing analytical model predictions towards high-fidelity simulation solutions via machine learning
Institute of Materials Mechanics, Helmholtz-Zentrum Hereon

14:10-14:25 S. Alameddin, J. Herb, R. Pereira Alessio, F. Fritzen
Simulation and experimental validation of residual stresses in laser-generated composite materials (SimKom)
Data Analytics in Engineering, University of Stuttgart

14:25-15:30 **Poster Session, including Coffee break (via GatherTown)**

15:30-15:45 D.K. Klein, M. Fernández, R.J. Martin, P. Neff, O. Weeger
Polyconvex anisotropic hyperelasticity with neural networks
Cyber-Physical Simulation Group, Technical University of Darmstadt

15:45-16:00 L. Dyckhoff, N. Huber
Predicting the Yield Surface of Nanoporous Metals using Data-Driven Modeling based on Machine Learning techniques
Hamburg University of Technology & Helmholtz-Zentrum Hereon

16:00-16:15 P. Weber, J.Geiger, W.Wagner, S.Freitag
Incoorporating physical restrictions by constraint optimization techniques for ANN-based hyperelastic material modeling
Institute for Structural Analysis, Karlsruhe Institute of Technology

16:15-16:30 T. F. Korzeniowski, K. Weinberg
Data-driven finite element computation of open-cell foam structures
Chair of Solid Mechanics, University of Siegen

16:30-16:45 S. Keshav, F. Fritzen, M. Kabel
Hadamard jump inspired composite boxels in FFT-based
Data Analytics in Engineering, Institute of Applied Mechanics, University of Stuttgart

16:45-17:00 **Concluding Remarks / Next Steps**

17:00-18:00 **Poster Session, including Christmas get-together (via GatherTown)**

7th GAMM AG Data Workshop 2021

List of Participants

- Shadi Alameddin, University of Stuttgart
- Renan Pereira Alessio, University of Stuttgart
- Heiko Andrä, Fraunhofer ITWM, Kaiserslautern
- Frederic E. Bock, Helmholtz-Zentrum Hereon
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1 Fracture network detected with X-Ray Computed Tomography (μXRCT)

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Fracture network in various kind of materials has been studied in many directions in recent years. It is well known that single fractures or multiple connected/disconnected fractures affect material properties such as stiffness, hydraulic permeability, thermal conductivity etc. significantly with consequences for various applications such as oil/gas production [1,2,3]. In order to understand effects of fractures networks on material properties, small-scale image-based characterization techniques like μXRCT became standard experimental approaches. X-Ray Computed Tomography provides a non-invasive insight into materials on the micro- or pore-scale level of porous materials and allow for the analysis of structural information of the fracture network topology. However, in image processing, clustering a thin and long, i.e. high aspect ratio structure of a fracture from a XRCT data set is demanding. Reasons are, bellow others, the low absorption contrast of cracks caused by the limitation of spatial resolution and low signal-to-noise ratio [4]. Therefore, we discuss fracture networks obtained with 5 different segmentation methods based on a XRCT data set of thermally induced fracture networks in Carrara marble [5]. In this comparison, three conventional methods such as Local Threshold (LT), Sato and Chan-vese (CV) were adopted. In addition, two Machine Learning-based approaches, such as Random Forest (RF) and 2D U-net method, were employed. Our study showed that the 2D U-net method outperformed the others in terms of segmentation quality and computational efficiency. In addition, the U-net method was able to provide proximate porosity compared to experimental measurement.

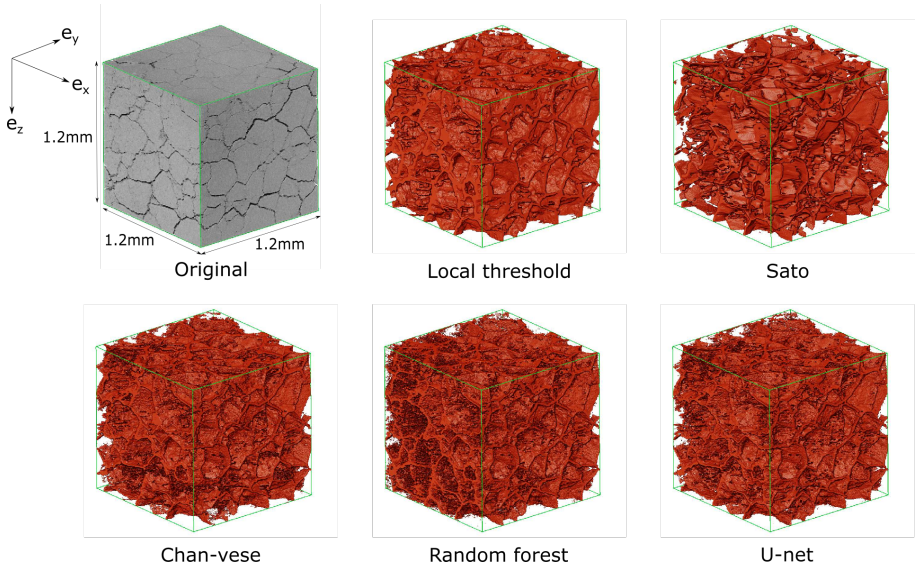

Figure 1: A comparison of segmented fractre networks obtained from 5 different segmentation methods

References

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[3] A. Suzuki et al. [2020]: "Inferring fracture forming processes by characterizing fracture network patterns with persistent homology", Computers & Geosciences 143, 104550, doi:10.1016/j.cageo.2020.104550

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[5] M. Ruf, H. Steeb [2020]: "Micro-XRCT data set of Carrara marble with artificially created crack network: Fast cooling down from 600°C", doi:10.18419/DARUS-682

2 New Experimental Characterisation of Cable Systems

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Large capital investments are being made on cable systems especially in the automotive field. Due to the strong growth in the digitalisation of vehicles, a considerable increase in the number of cables can be seen in them. Cable bundles and harnesses are used for better cable management in these vehicles. Each cable bundle is made up of various cables and each of these cables are complex components consisting of a multi-layer structure made up of various materials. In order to characterise these cable bundles, the prediction of the effective mechanical properties of the system as a whole is focussed on.

Due to their construction, the interaction between the different components in a cable bundle leads to deviation from classical material behaviour [1]. The bending movement induces friction between the cables resulting in non-linearity effects as well as coupling between the bending and torsion load cases. These non-linearity effects have to be analyzed on the basis of the data obtained in the experiments that will later be used as training for a neural network. The use of the neural network is due to the diversity of cable structures and compositions, such as the diameter, the number of cables, the cable types, materials and mechanical parameters of the individual components. These parameters are then used as input parameters for the neural network and finally to develop a data-based model of cable system that predicts the mechanical properties of cable systems.

For this purpose, a new test rig has been designed and built, allowing the implementation of the decoupled load cases: bending, torsion and uniaxial tension, as well as their superposition on the slender flexible structures. A nonlinear pure bending for a single cable has been already performed at the institute and further experiments will be perfomed on a system of cables.

Reference

[1] V. Dörlich, S. Diebels and J. Linn [2015]: "Investigation of elastoplastic effects of cables under large spatial deformation", PAMM Proc. Appl. Math. Mech. **1**, 185–186

3 Convolutional Neural Networks - how to make them work for periodic image data

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For high-performance materials the desired properties are induced by the microstructure. Assuming periodic boundary conditions of the microstructure, the material is characterized by a single frame of the microstructure, the representative volume element (RVE). Computing the response of such microstructure remains computationally costly, despite recent improvements using FFT based schemes [1]. In order to improve computational efficiency, machine learning models are deployed. Recent studies successfully predicted the effective response for periodic microstructures with descriptor based approaches or with reduced coefficients/principal components of the two point correlation function [2], however, it has been shown that the accuracy of these approaches is limited.

On the quest for an improved prediction we manually engineered new features to better quantify the microstructure geometry. Unsatisfied by the improvement we deployed convolutional neural networks, which discover high-level features based on the available training data. Ideally the convolutional neural network should be frame invariant with respect to translation to suit the periodic boundary conditions (Figure 1), which is not unconditionally given for general convolutional neural networks [3]. Methods to ensure frame invariance are e.g. mapping to Fourier space via the Fast Fourier transform, which induces periodic boundary conditions, or the deployment of a particular neural network architecture we developed and deployed, ensuring a priori frame invariance.

Ultimately we developed a hybrid model which captures high-level features from a convolutional branch, and incorporates the frame invariant features we engineered, leading to a significant improvement in prediction accuracy. The deployed model does not strictly guarantee frame invariance in order to balance computational cost and accuracy. We show that the sacrificed accuracy by allowing minor frame dependence is negligible.

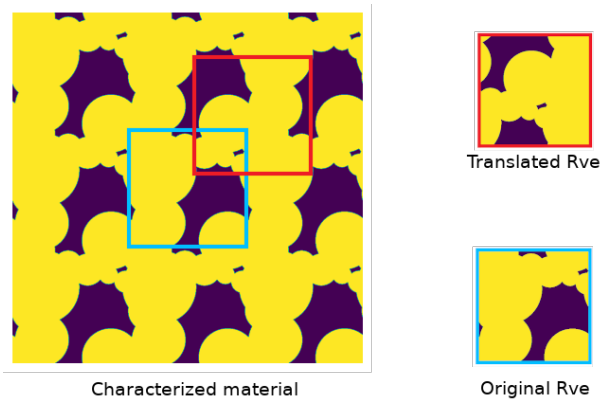

Figure 1: The material represented by the original RVE (light blue box) can also be represented by a different RVE (red box), leading to completely different images.

References

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4 Hybrid modelling: Combining physics-based and data-driven modelling by enhancing analytical model predictions towards high-fidelity simulation solutions via machine learning

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For predictions within the areas of materials mechanics along the process-structure-property-performance chain, the utilization of physical laws offers the potential to substantially enhance prediction performance, as opposed to using only data. On the one hand, models based on fundamental and well-established physical laws can easily exhibit deviations to the anticipated solution due to involved simplifications, assumptions and miss-calibrations. On the other hand, models only based on data can map complex relationships without the need to explicitly formulate or calibrate physical equations; however, they can require a significant amount of good-quality data to represent the problem at hand, which can seem redundant when involved physical relationships are already known.

Via a hybrid model consisting of both physics-based and data-driven modelling, the weaknesses of each approach can be compensated by exploiting each model's respective advantages. Concretely, we propose a hybrid model where a physics-based analytical model shows discrepancies to the anticipated solution and is corrected by a data-driven model that maps those discrepancies. In a case-study on predictions of residual stresses induced by Laser Shock Peening , a physics-based semi-analytical model is corrected by an artificial neural network towards solutions from high-fidelity finite element simulations, while the computational efficiency of the semi-analytical model is maintained. Additionally, the trained process parameter space can be expanded via physical normalization of inputs and outputs. As a result, the hybrid model outperforms physics-based and data-driven models showing considerably lower prediction errors and an enhanced range of applicability, especially when the available data is scarce.

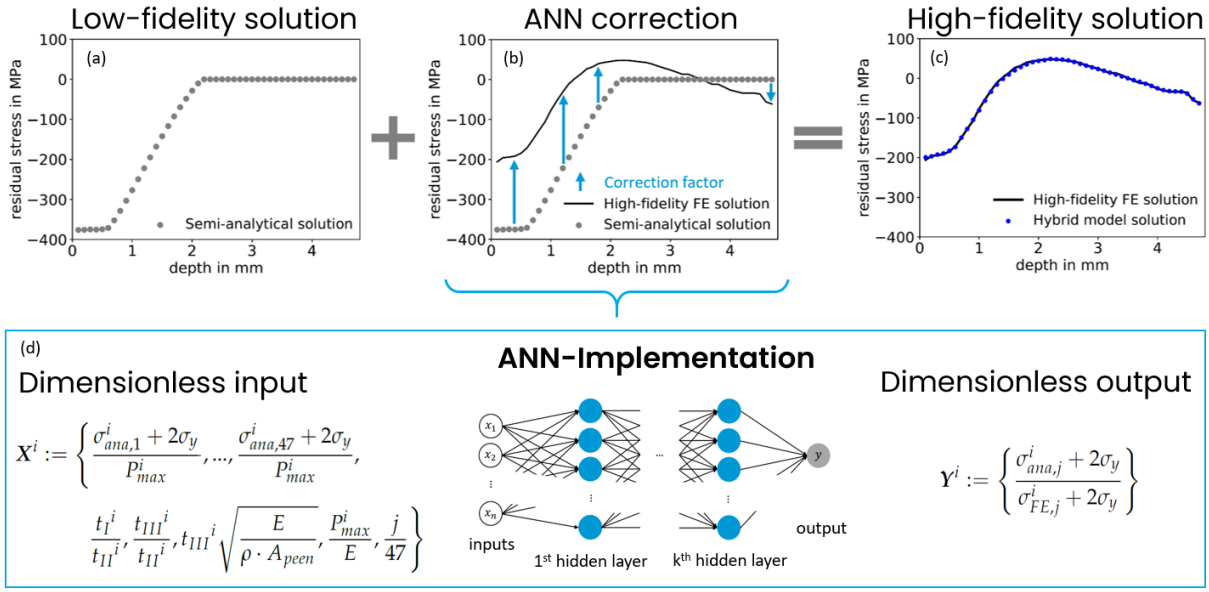

Figure 1: Schematic of hybrid model predictions of residual stress distribution induced by Laser Shock Peening: (a) Residual stress predictions by the semi-analytical model corrected towards (b) high-fidelity finite element solutions via correction factors approximated by an artificial neural network (ANN), yielding (c) the anticipated high-fidelity solution with hybrid model predictions. The implementation of the ANN with respect to its dimensionless inputs and outputs is shown in (d).

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5 Simulation and experimental validation of residual stresses in laser-generated composite materials (SimKom)

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This work presents a multiscale simulation framework that will be used for the simulation and experimental validation of eigenstresses in composite materials generated via laser-dispersion. These materials are obtained by adding tungsten carbide particles into the melt pool of a base metal to generate surface coatings. Such coatings are used to boost wear-resistance, more precisely to protect metallic surfaces against abrasion, erosion or corrosion. The coating significantly extends the part's lifetime due to the outstanding material characteristics of the locally produced metal matrix composite (MMC). Eigenstresses, which are the residual stresses left in the MMC material after the coating process, shall be investigated and predicted within the framework of this project and their effect on the lifetime shall be estimated.

Computational homogenization is employed to predict the thermo-mechanical response of heterogeneous structures. In such schemes, the constitutive response of every integration point in the macro scale is obtained by solving a boundary value problem on a representative volume element (RVE) with boundary conditions from the corresponding integration point. Direct numerical simulation (DNS) of RVE response, which can be seen in FE^2 context, is computationally demanding. In contrast, reduced order models (ROM) and data-driven surrogate models provide an appealing and efficient alternative to DNS. Hence, our goal is to use reduced order models and machine learning to tackle challenging multi-scale thermo-mechanical problems. In this context an interface to LS-DYNA was developed to allow for direct integration of surrogate models written in Python and C++ [1]. Then various data-driven models to predict the effective behaviour on the microscale were invistigated [2]. In addition, the established isothermal nonuniform transformation field analysis (NTFA) from [3] is being extended toward anisothermal settings with temperature dependent material parameters.

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6 Polyconvex anisotropic hyperelasticity with neural networks

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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.

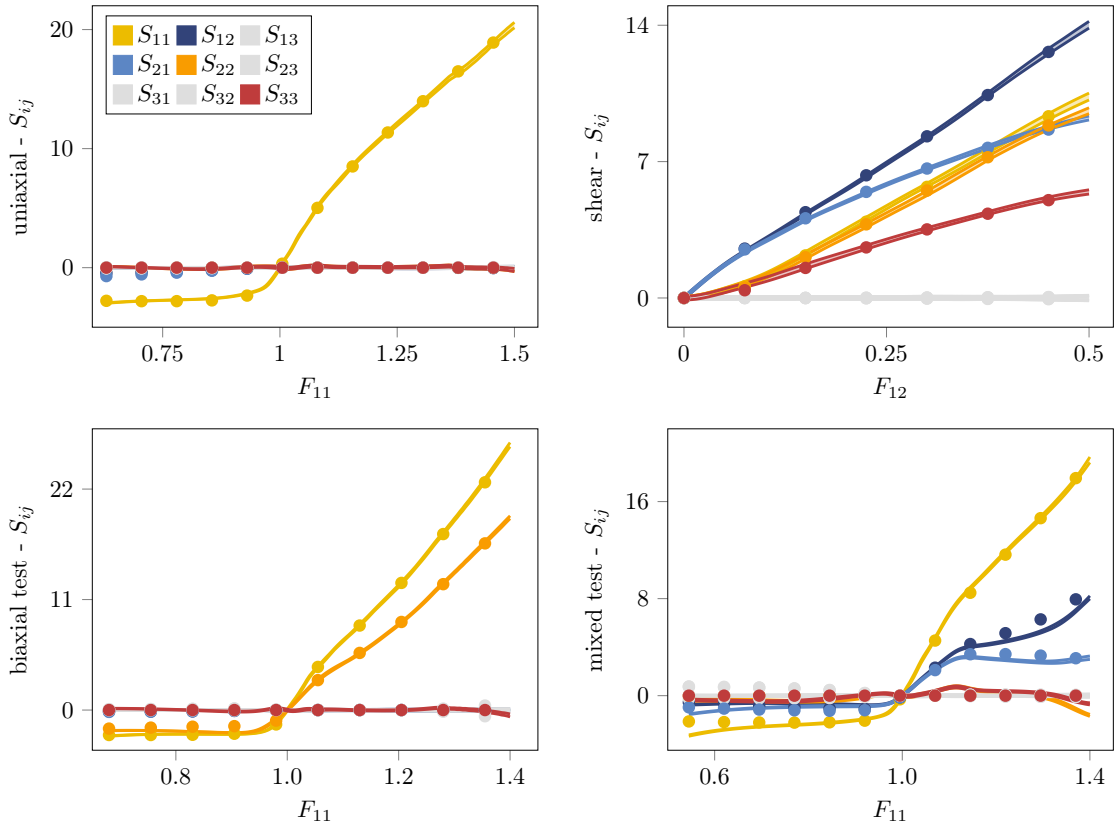

Figure 1: Evaluation of the deformation gradient based model for the cubic BCC cell. Points depict the simulation data, lines depict the calibrated model, stress in [hPa].

References

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7 Predicting the Yield Surface of Nanoporous Metals using Data-Driven Modeling based on Machine Learning techniques

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Nanoporous metals made by dealloying are multiscale and light weight materials consisting of nanoscaled ligaments with high strength, which themselves can exhibit an additional level of hierarchy. Due to the complex structure it is a challenge to predict the strength of such materials on the macroscale, especially regarding complex load cases and the loading history.

Here FE Modeling is combined with different machine learning techniques to predict the yield surface as a first step towards a constitutive surrogate model to describe the elastic-plastic behaviour of the lower levels of hierarchy. Two simplified representative volume elements, a diamond and a kelvin cell, made of beam elements were built using NPGModeler.[1] The elastic behaviour of both models follows the constitutive law of linear elasticity with cubic anisotropy. With that the yield strength under multiaxial loading is determined from numerical calculation and subsequently used as training, test and validation data for machine learning algorithms such as support vector machines and artificial neural networks (ANN). In addition the Deshpande-Fleck model for isotropic solid foams[2] is compared to the numerical yield surface and used 1to implement a hybrid ANN. These models enable the prediction of the yield surface in three dimensional stress space with an average relative approximation error of around 1 % depending on the amount of traning data.

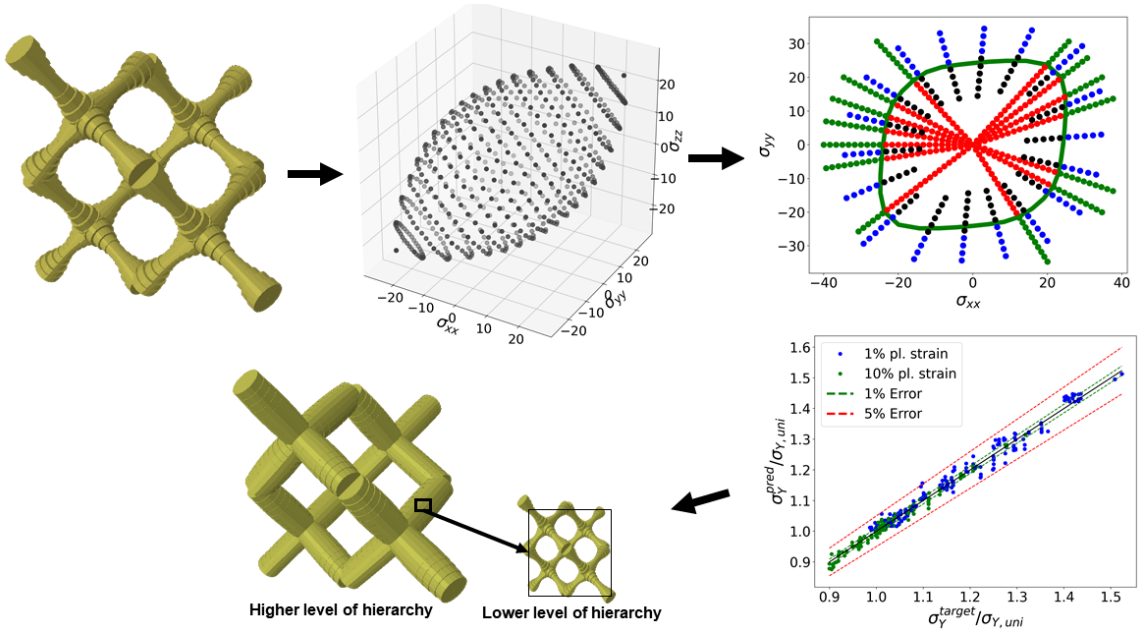

Figure 1: Predicting the elastic-plastic behaviour of lower hierarchy levels using FE Modeling and machine learning algorithms.

References

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[2] V.S. Deshpande, N.A. Fleck [2000]: „Isotropic constitutive models for metallic foams“, Journal of the Mechanics and Physics of Solids **48**, 1253–1283

8 Incoorporating physical restrictions by constraint optimization techniques for ANN-based hyperelastic material modeling

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Developing purely data based material models by means of artificial neural networks (ANNs) has gained more popularity in the last years, as can be seen by the growing number of publications. One disadvantage using ANNs is the lack of physical restrictions, which are in general not considered within the training process. This leads to a huge amount of data needed to learn these restrictions indirectly. While some contributions aim to solve this issue by defining specific ANN architectures, we consider physical restrictions in the ANN training with constraint optimization techniques. This allows to use classic ANN architectures, while the physical restrictions can be flexibly specified according to the desired material behavior.

In [1], the authors restricted the ANN training by enforcing energy conservation, isotropy and a stress-free rigid-body motion in order to simulate hyperelastic material behavior. Within numerically challenging finite element calculations, e.g. a bifurcation problem using a shell formulation which is able to use 3d material models [2], the feasibility of the proposed method is shown. On the basis of sparse real world data [3], meaning only 121 samples in a 6d strain/stress-component space, a numerically stable material model can be generated. The proposed physically enhanced ANN training outperforms state-of-the-art techniques, which e.g. enrich the sample set by adding synthetic samples through reference frame rotation, with respect to numerical stability and convergence behavior, see Figure 1.

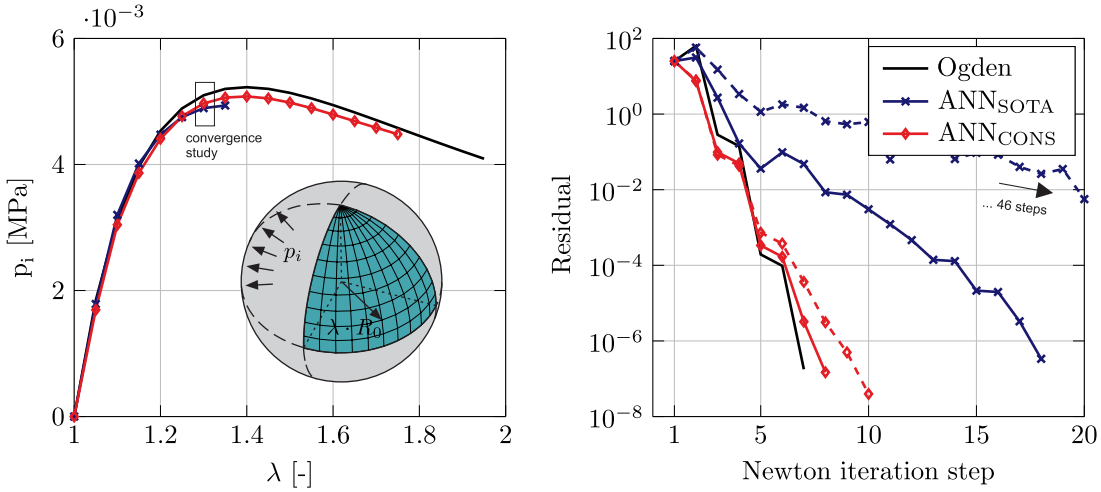

Figure 1: FE example according to [1]: rubber balloon with initial radius R_0 under inner pressure p_i. Left: load-stretch-curve, right: convergence behavior for load step six of the global Newton iteration. Comparison of ANN trained with constraints (CONS) a state-of-the-art ANN model (SOTA) with synthetic samples and L2-regularization and an analytical Ogden reference material.

In this contribution, we focus on the numerical implementation of various constraints within ANN training. This includes the performance of penalty and exact penalty methods in combination with ANN training algorithms, as well as studies on the effect of enhanced ANN training with respect to small sample sizes and noisy data.

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[3] L.R.G. Treloar [1944]: "Stress-strain data for vulcanized rubber under various types of deformation", Rubber Che, Technol **17**(4), 813–825

9 Data-driven finite element computation of open-cell foam structures

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In the data-driven finite element analysis the constitutive material modeling is eluded and experimental data are directly employed as an input for computational analysis instead. Therefore there is no need for an explicit constitutive relationship. Typically it is intended to extract these data from experimental tests. However, until now, artificial data sets are often gained by known material laws that are then forgotten for simulations. Our contribution focuses on the meaningful generation of numerical data via representative volume elements (RVEs). Polyurethane foam RVEs are gained from an in-house software package developed in the recent years. By applying simple loading states we can generate a database that describes the macroscopic behavior of the foam in a data-driven finite element analysis. After starting with a small database, regions can be identified where more data is needed. The proposed algorithm is very similar to a FE^2 computation then.

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nite element computations, Computer Methods in Applied Mechanics and Engineering 379 (2021) 113740.

10 Hadamard jump inspired composite boxels in FFT-based homogenization

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In recent years, computational homogenization techniques have helped perform concurrent multi-scale simulations (e.g., FE2) in view of scale-bridging applications. For discrete, voxelized microstructural data they have become the gold standard to perform high-fidelity multi-scale analysis despite some disadvantages close to material boundaries and are computationally overly expensive. The computational complexity of simulations operating on such three-dimensional high-resolution voxel data comprising billions of unknowns induces the need for algorithmically and numerically highly efficient solvers at the microscale. In this work, we use a specific Fast Fourier Transform (FFT) based technique called Fourier-accelerated nodal solvers (FANS) to efficiently perform numerical homogenization of heterogeneous microstructures for linear and nonlinear multi-physical problems operating on high-resolution regular grids. The inability of binarized microstructures to capture smooth material interfaces accurately along with the need for complexity reduction motivates a special local coarse-graining technique called composite voxels which have been shown to work exceedingly well for a variety of FFT based discretization techniques including FANS. These composite voxels are supervoxels with a theory-inspired constitutive model that is built on established mechanical principles. They have been shown to significantly improve local field quality at a fraction of the computational cost. Our contribution comprises the generalization towards composite boxels that can be nonequiaxed. Therefore, a novel image-based normal detection algorithm is developed which leads to excellent accuracy in academic benchmarks as well as in realistic simulations. We highlight points for an efficient implementation, numerical results of the composite boxels alongside methodological enhancements for materially and geometrically linear/nonlinear multiphysics problems.

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