Challenges and Perspectives in Data-driven Modeling

GAMM AG Data Workshop 2018

May 03–04, 2018

Leuphana University of Lüneburg
Helmholtz-Zentrum Geesthacht

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

2 Objectives

- To discuss the state of the art and recent trends in computational and experimental research
- To plan the AG Data activities
- Explore possible collaborations with DGM
- Lab tours with focus on modern experimental techniques for microstructure characterization at the Helmholtz-Zentrum Geesthacht

3 List of Participants

- M.Sc. Masoud Abbaszadeh, Helmholtz-Zentrum Geesthacht
- M.Sc. Frederic E. Bock, Helmholtz-Zentrum Geesthacht
- Prof. Dr.-Ing. Christian J. Cyron, Hamburg University of Technology
- Prof. Dr.-Ing. Stefan Diebels, Saarland University
- M.Sc. Robert Eggersmann, RWTH Aachen University
- Dr.-Ing. Rainer Falkenberg, Bundesanstalt für Materialforschung und- prüfung (BAM)
- Dr.-Ing. Dipl.-Math. techn. Felix Fritzen, University of Stuttgart
- M.Sc. Christian Gebhardt, RWTH Aachen University
- Prof. Dr. Alexander Hartmaier, Ruhr Universität Bochum
- M.Sc. Reza Hassani, University of Stuttgart
- M.Sc. Jan Herrnring, Helmholtz-Zentrum Geesthacht
- Prof. Dr.-Ing. Norbert Huber, Helmholtz-Zentrum Geesthacht
- M.Sc. Sören Keller, Helmholtz-Zentrum Geesthacht
- Prof. Dr.-Ing. Benjamin Klusemann, Leuphana University Lüneburg & Helmholtz-Zentrum Geesthacht
- M.Sc. Tim Fabian Korzeniowski, University of Siegen

- M.Sc. Stephan Kreis, Karlsruher Institute of technology
- M.Sc. Oliver Kunc, University of Stuttgart
- Prof. Dr. Erica Lilleoden, Helmholtz-Zentrum Geesthacht
- Prof. Dr. Rolf Mahnken, Paderborn University
- Prof. Dr. mont. Christian Motz, Saarland University
- Dr.-Ing. Lu Trong Khiem Nguyen, University of Stuttgart
- Prof. Michael Ortiz, PhD, California Institute of Technology & University of Bonn
- Dr.-Ing. Aruna Prakash, TU Bergakademie Freiberg
- M.Sc. Benedikt Prifling, Ulm University
- M.Sc. Dennis Rapp, University of Stuttgart
- M.Sc. Syed Hasan Raza, Leuphana University of Lüneburg
- M.Sc. Claudia Richert, Helmholtz-Zentrum Geesthacht
- Prof. Dr. Stefan Sandfeld, TU Bergakademie Freiberg
- Dr.-Ing. Ingo Scheider, Helmholtz-Zentrum Geesthacht
- M.Sc. Frederik Scherff, Saarland University
- M.Sc. David Uribe, University of Stuttgart
- M.Sc. Daniel Wicht, Karlsruher Institute of Technology

4 Schedule

Thursday, 03.05.2018 (Central building Leuphana University Lüneburg, C40.704)

10:00 – 11:30	city tour Lüneburg (meeting point Tourist Information (Rathaus/Am Markt))
12:00	**Lunch**
12:50 – 13:00	Opening
13:00 – 13:45	N. Vajragupta, D. Reimann, H. ul Hassan, A. Hartmaier (keynote lecture) *Micromechanical modeling of plasticity and damage in realistic microstructures* Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum
13:45 – 14:10	B. Prifling, D. Westhoff, V. Schmidt *Quantitative analysis and stochastic 3D modeling of tomographic image data for electrodes in lithium-ion batteries* Institute of Stochastics, Ulm University
14:10 – 14:35	E. Lilleodden, K. Hu, M. Ziehmer *Correlating 3D structural characteristics to micro-mechanical behavior of nanoporous gold* Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht
14:35 – 15:00	C. Richert, N. Huber *Skeletonization, Geometrical Analysis and Finite Element Modeling of Nanoporous Gold Based on 3D Tomography Data* Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht
15:00 – 15:30	**Coffee break**
15:30 – 15:55	D. Uribe, H. Steeb *Experimental analysis of multiphase ow and solute transport in porous media using SXRCT*

	Institute of Mechanics (CE), University of Stuttgart
15:55 – 16:20	C. Motz and J. R. Velayarce *Influence of grain boundaries on fatigue damage evolution studied by micro fatigue tests* Department of Material Science and Engineering, Saarland University
16:20 – 16:45	F. Scherff, S. Scholl, K. Srivastava, S. Diebels *Simulation of dual-phase steel based on real and virtual 3D microstructures* Lehrstuhl für Technische Mechanik, Saarland University
16:45 – 17:10	M. Schneider, D. Wicht *On polarization-based schemes for FFT-based computational homogenization of inelastic materials* Chair for Continuum Mechanics, Institute of Engineering Mechanics, Karlsruhe Institute of Technology
17:10 – 17:25	S. Sandfeld *Presentation DGM Arbeitskreis "3D Data Science" (Fachausschuss Materialographie)*
17:25 – 18:15	Discussion Collaboration DGM / Further Steps GAMM Activity Group
19:00	**Workshop-Dinner (Mälzer Brau- und Tafelhaus, Lüneburg)**

Friday, 04.05.2018 (HZG Hörsaal, building 27)

08:30	Transfer to Helmholtz-Zentrum Geesthacht (pick-up point Best Western Plus Residenzhotel Lüneburg, Munstermannskamp 10, 21335 Lüneburg)
09:15 – 10:00	Lab tour **Solid State Joining Processes (Materials Mechanics)**
10:15 – 11:00	M. Ortiz (keynote lecture) *Data-Driven Computing* California Institute of Technology, USA & Hausdorff Center for Mathematics, University of Bonn
11:00 – 11:25	K. Nguyen, M. Rambausek, M.-A. Keip *A variational framework for data-driven computational mechanics applied to elasticity* Chair of Material Theory, University of Stuttgart
11:25 – 11:50	S. Sandfeld *Data mining in small-scale plasticity* Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg
11:50 – 12:15	F. Fritzen, O. Kunc *Data-assisted surrogate modeling of nonlinear solids* Emmy-Noether-Group EMMA – Efficient Methods for Mechanical Analysis, University of Stuttgart
12:15 – 12:30	Final discussions
12:30 – 13:15	**Lunch**
13:15 – 14:00	Lab tour **Magnesium Innovation Centre MagIC**
14:00 – 14:30	Lab tour **Joining and Assessment (Materials Mechanics)**
14:30	End of the workshop – Transfer to Hamburg-Nettelnburg and Lüneburg

5 Abstracts

5.1 Micromechanical modeling of plasticity and damage in realistic microstructures

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Micromechanical modeling is applied to describe plastic deformation and damage in realistic microstructures. The micromechanical method described here is based on three main constituents: (i) generation of 'synthetic' material microstructures in form of representative volume elements (RVE) (ii) implementation and application of crystal plasticity and damage models, and (iii) homogenization of the results into macroscopic constitutive rules. The approach is applied to two cases:

Micromechanical modeling of the influence of microstructure of DP600 steel on sheet metal forming processes. The microstructure is quantitatively characterized to gain relevant statistical information of all important microstructural features such as phase volume fractions, grain size distributions and orientation distributions of each constituent. The obtained results are used to generate an RVE by a combination of particle simulation methods with radical Voronoi tessellation. Finite element simulations with a nonlocal crystal plasticity model are then conducted under various loading conditions to investigate the corresponding mechanical responses. Finally, the mechanical behavior of the RVE is homogenized in form of a simplified flow rule.

Homogenization of microstructural damage evolution with machine learning algorithms. Micromechanical models are in general able to describe microstructural influences, such as texture and grain size distribution, on damage evolution. A homogenization from the micro to the macro scale is, however, conceptually demanding. Hence, a new approach involving machine learning algorithms is suggested. In this work, numerical data based on RVE simulations is used to train the machine learning algorithm, which in turn describes damage evolution as function of loading conditions and microstructure.

5.2 Quantitative analysis and stochastic 3D modeling of tomographic image data for electrodes in lithium-ion batteries

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Lithium-ion batteries play a major role in a large number of applications ranging from portable devices to electric vehicles. In recent years, lithium-ion batteries became more and more important due to their preferable electrochemical properties as for example a relatively high energy density. It is well known that the morphology of the electrodes mainly influences the overall battery performance. Therefore, a deeper understanding of the microstructure of cathodes as well as anodes is an important task with regard to the optimization of functionality.

The first part of this talk will focus on eight experimentally manufactured cathodes described in [1]. With the aid of synchrotron tomography and several image processing techniques we are able to obtain phase- as well as particle-segmented image data, which provide valuable information regarding the electrochemical performance. Furthermore, the combination of parametric probability distributions and least-squares regression is a powerful tool in order to predict the distributions of microstructural characteristics as a function of the compaction load [2]. The second part of the talk deals with the algorithmic segmentation of defective particle systems [3]. Finally, we present several stochastic 3D microstructure models for cathodes as well as anodes in lithium-ion batteries, see e.g. [4], [5], [6] and [7]. This allows us to describe the 3D morphology of battery electrodes using only a few parameters. Additionally, a large number of virtual but realistic microstructures of electrodes can be simulated, which can be used for electrochemical modeling and simulation [8,9].

References

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[2] K. Kuchler, B. Prifling, D. Schmidt, H. Markötter, I. Manke, V. Knoblauch, V. Schmidt [2018]: "Analysis of the 3D microstructure of experimental cathode films for lithium-ion batteries under increasing compaction", Journal of Microscopy (submitted)

[3] D. Westhoff, D.P. Finegan, P.R. Shearing, V. Schmidt [2018]: "Algorithmic structural segmentation of defective particle systems: A lithium-ion battery study", Journal of Microscopy **270**, 71–82

[4] D. Westhoff, I. Manke, V. Schmidt [2018]: "Generation of virtual lithium-ion battery electrode microstructures based on spatial stochastic modeling", Computational Materials Science (submitted)

[5] J. Feinauer, T. Brereton, A. Spettl, M. Weber, I. Manke, V. Schmidt [2015]: "Stochastic 3D modeling of the microstructure of lithium-ion battery anodes via Gaussian random fields on the sphere", Computational Materials Science **109**, 137–146

[6] D. Westhoff, J. Feinauer, K. Kuchler, T. Mitsch, I. Manke, S. Hein, A. Latz, V. Schmidt [2017]: "Parametric stochastic 3D model for the microstructure of anodes in lithium-ion power cells", Computational Materials Science **126**, 453–467

[7] K. Kuchler, D. Westhoff, J. Feinauer, T. Mitsch, I. Manke, V. Schmidt [2018]: "Stochastic model for the 3D microstructure of pristine and cyclically aged cathodes in Li-ion batteries", Modelling and Simulation in Materials Science and Engineering **26**, 035005

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[9] S. Hein, J. Feinauer, D. Westhoff, I. Manke, V. Schmidt, A. Latz [2016]: "Stochastic microstructure modeling and electrochemical simulation of lithium-ion cell anodes in 3D", Journal of Power Sources **336**, 161–171

5.3 Correlating 3D structural characteristics to micro-mechanical behavior of nanoporous gold

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The mechanical behavior of NPG has been shown to be strongly dependent on its average ligament width, with local stresses approaching the theoretical strength of gold, underscoring the "smaller is stronger" paradigm. Such size-dependent strength can be exploited in NPG through targeted an-nealing in order to tailor the structural length-scales. Yet strong deviations from classical laws for cellular structures have been found for NPG, pointing to the need for developing new scaling laws for the prediction of mechanical properties as a function of structural length. This in turn is reliant on a more detailed investigation of the 3D network structure and crystallographic domain sizes, and a better understanding of the underlying structure-property relations governing mechanical response. By employing a combination of high-resolution tomographic characterization, micro-Laue diffraction and in situ micromechanical testing, the structure-property relations and mechanisms of deformation of this NPG have been explored and quantified. Using focused ion beam (FIB) based tomography applied to as-dealloyed and isothermally annealed NPG samples, we show that the ligament width distributions coarsen in a sufficiently self-similar, time-invariant manner, while the scaled connectivity density shows a self-similar ligament network topology, best described as a load-bearing ring structure. Finally, insights from micro-Laue diffraction experiments point to the role of structural length-scale on the distribution of dislocation structures and mechanisms of de-formation.

5.4 Skeletonization, Geometrical Analysis and Finite Element Modeling of Nanoporous Gold Based on 3D Tomography Data

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Various modeling approaches simplify and parametrize the complex network structure of nanoporous gold (NPG) 1 for studying the structure-property relationship based on artificially generated structures. This paper presents a computational efficient and versatile FEM beam model that is based on skeletonization and diameter information derived from the original 3D FIB-SEM tomography data of NPG 2. The geometrical skeleton network is thoroughly examined for a better understanding of the NPG structure. A skeleton FEM beam model is derived that allows predicting the macroscopic mechanical behavior of the material 3. Comparisons between the mechanical response of this skeleton beam model and a solid FEM model are conducted. Results showed that the biggest-sphere diameter algorithm implemented in the open-source software FIJI, commonly used for geometrical analysis of microstructural data, overestimates the diameter of the curved NPG ligaments. The larger diameters lead to a significant overestimation of macroscopic stiffness and strength by the skeleton FEM beam model. For a parabolic shaped ligament with only 20% variation in its diameter a factor of more than two was found in stiffness. It is concluded that improved algorithms for image processing are needed that provide accurate diameter information along the ligament axis.

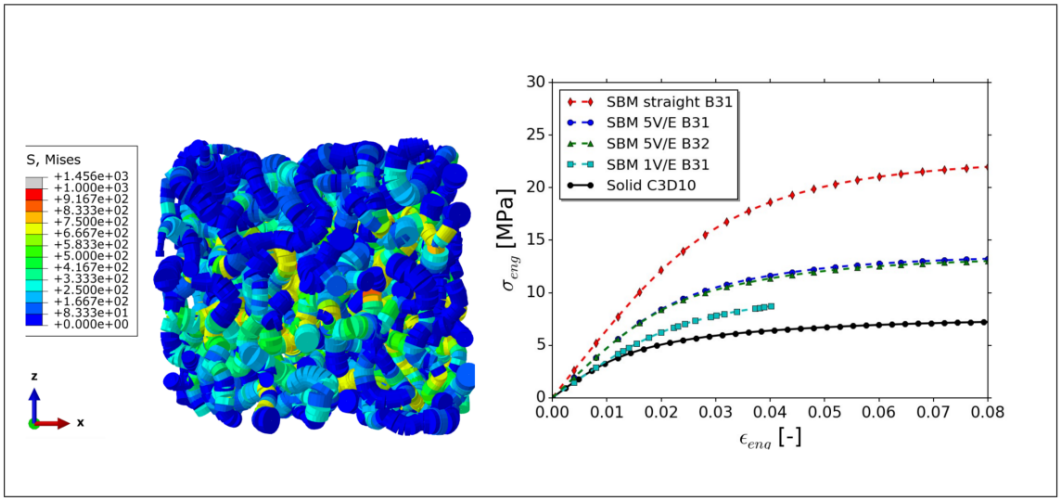

Figure 1: Skeleton FEM beam model of the NPG structure compressed to 8% macroscopic strain (left); Macroscopic stress-strain response under compressive loading for solid FEM model consisting of C3D10 elements (black line) and skeleton FEM beam models (SBM) (dashed lines). For the skeleton FEM beam model, the curves for different discretization approaches are shown: straight junction-junction connection (red), approximately five voxel per element (5V/E) with B31 beam elements (blue), or B32 beam elements (green), and the finest approach with one voxel per element (1V/E) (cyan)

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5.5 Experimental analysis of multiphase flow and solute transport in porous media using SXRCT

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Synchrotron-based X-Ray Computed Tomography (SXRCT) has various major advantages over classical small vacuum tube sources. Synchrotron radiation has a parallel ray configuration, a monochromatic spectrum, the coherence of the rays, and the magnification is only limited by the optics of the used optical magnification. The greatest feature of synchrotron radiation for *in-situ* experiments is the available high flux in combination with ultra-fast high-resolution CMOS cameras. Some synchrotron beamlines have been able to capture ultra-fast dynamic experiment at acquisition frequencies of upto 20 Hz [1]. Here, 20 Hz means 20 full 3-dim scans per second.

In our contribution, we show the latest results of our solute transport experiments performed at the Diamond Light Source, Didcot, UK. The investigated porous medium is composed of a in-house developed flow cell, cf. [3], filled with mono-disperse glass beads. In the primary imbibition step, the artificial porous medium is saturated with fluorinert. Afterwards, in the drainage step, water is injected at different flow rates, breaking through the fluorinert creating a tortuous connected flow path. In a subsequent step, a water-based solution of 1 mol KI is injected into the pore space at different flow rates. We evaluate the different diffusion time scales found in the experiment as in [2].

We demonstrate a post processing strategy to handle large datasets. The amount of information generated from this experiment is in the order of 100's of terabytes, and accuracy of the image analysis has to be compromised for practical reasons, within reasonable boundaries. Furthermore, the diffusion characteristics can be derived from voxel values' histogram, facilitating the data analysis.

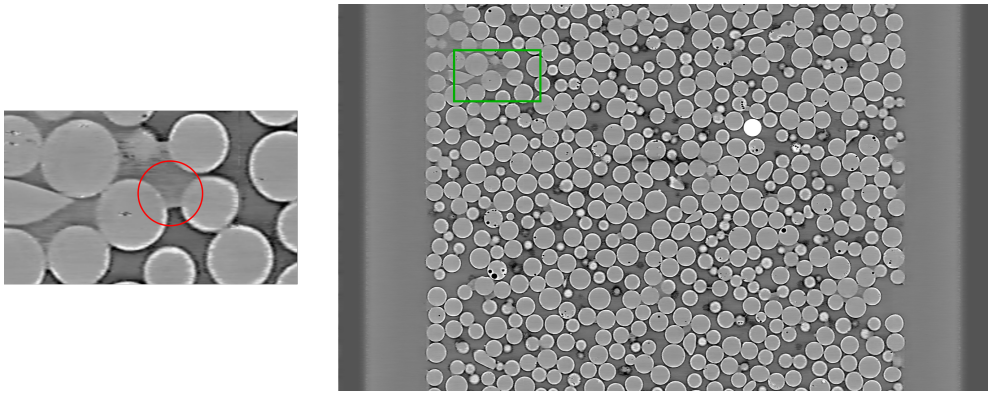

Figure 1: vertical cut of the porous medium in an intermediate time step. Flow direction is downwards.The circle in the left figure shows the interface between the fluorinert, glass beads and the water with a low KI concentration. In the right figure, the gradient in the KI concentration can't be directly seen, which motivates the use of histograms to evaluate the global concentration. The rectangle represents the area from which (left) was extracted.

References

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5.6 Influence of grain boundaries on fatigue damage evolution studied by micro fatigue tests

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The size of typical fatigue dislocation structures, e.g. persistent slip bands or cell structures, is in the order of micrometers. These structures are usually associated with local damage evolution and are limiting the lifetime of components. However, reducing the sample-size down into this regime raises questions about developing microstructures and damage. Also phase and grain boundaries may have a significant influence on deformation and damage initiation at the local scale.

Thus, the development of fatigue microstructures and the damage evolution will be studied by in-situ fatigue tests in the SEM on single and bi- crystalline micro-samples depending on specimen size, dislocation density and crystal orientation. The microstructure evolution is measured by electron channeling contrast and by high resolution electron backscatter diffraction (HR-EBSD), and post-mortem by transmission electron microscopy (TEM). Furthermore, local stresses (strains) are estimated by HR-EBSD and analysis of the Bauschinger effect. These measurements are supported by 3D discrete dislocation dynamics simulations (3D-DDD). This allows the correlation between microstructure and damage and the local loading of the sample.

In the case of grain boundaries incompatibilities in local stresses and strains are of interest as these are correlated with the damage evolution at the grain boundary. The main advantage of using micron-sized specimen is the knowledge of the local stresses and strains, which allows to associate changes in the stress vs. strain response with microstructural events.

The aim of the presentation is to understand the development of fatigue microstructures in dependence of the specimen size in order to predict the lifetime of miniaturized parts and components. Additionally, it will lead to a better understanding of the role of grain boundaries in fatigue damage evolution and can help to improve current models.

5.7 Simulation of dual-phase steel based on real and virtual 3D microstructures

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The mechanical properties of modern dual-phase (DP) steels are characterized by high strength, high work hardening and an elevated level of ductility. The main cause of these qualities is the microstructure, consisting of a soft ferrite matrix and a hard martensite phase embedded therein[1]. These properties make it desirable to also use dual-phase steels in the heavy plate steel sector, as they are already used in the automotive and aerospace industries for energy absorbing, strength-relevant structures.

The focus of this work is the development of an FE model to predict the deformation of DP steel based on three-dimensional microstructure data, incorporating the underlying mi rostru ture properties[2]. The relevant quantitative information on microstructures is acquired by means of serial section tomography[3]. As with any microstructure-based simulation, determining the size of the representative volume element (RVE) is essential for statistical independence. To this end, a method to determine the RVE size from experiments is presented and validated.

Based on this work, virtual microstructures are created in such a way that they are adapted to the real structure in their relevant geometric parameter. The simulated stress-strain-curves on these virtually generated microstructures agree well both with the experiments and the simulations on real microstructures, see Fig. 1. This method then enables the investigation of the mechanical properties as a function of microstructure.

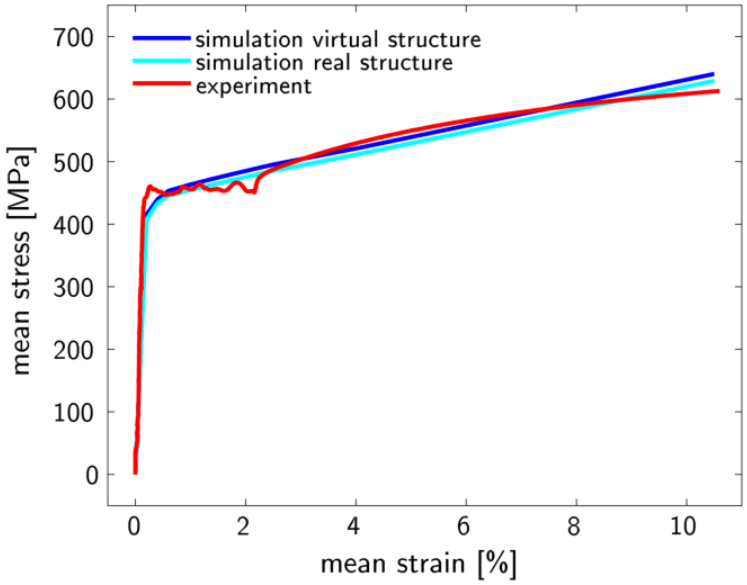

Figure 1: Comparison of simulated and experimental mean stress - mean strain - curves for a real and a virtual DP steel microstructure in uniaxial tensile test.

References

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5.8 On polarization-based schemes for FFT-based computational homogenization of inelastic materials

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Starting with the works of Moulinec and Suquet [1] in the 90s, FFT-based computational homogenization methods have gained much popularity for the prediction of effective material properties due to their computational efficiency. Based on the so-called basic scheme by Moulinec-Suquet, Eyre-Milton [2], Michel-Moulinec-Suquet [3] and Monchiet-Bonnet [4] introduced formally similar accelerated schemes which exhibit faster convergence rates than the basic scheme for composites with high contrast.

Unfortunately, these polarization-based methods suffer from two handicaps when applied to non-linear problems. Firstly, the optimal choice of algorithm parameters is only known for the linear case. Secondly, in its original version [2] each iteration of the polarization scheme requires solving a nonlinear system of equations for each voxel. In this work, we overcome both difficulties for small-strain viscoplastic materials. In particular, we show how to avoid solving the non-linear system. The convergence behavior of the scheme is compared to the basic scheme and other accelerated gradient methods, e.g. [5], based on numerical demonstrations.

References

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5.9 Data-Driven Computing

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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.

5.10 A variational framework for data-driven computational mechanics applied to elasticity

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A boundary value problem of continuum mechanics consists of three ingredients: The compatibility condition, the conservation laws, and the material laws that relate the work conjugates such as the strain and the stress. The material laws are usually expressed in terms of a functional relationship that fits empirical observations based on experimental data. It is sometimes difficult to calibrate a material model to fit the collected data for sophisticated material behaviors. In the data-driven computation such functional relation is replaced with an abundant collection of material data and such problem is addressed by Kirchdoerfer and Ortiz resorting to a least-squares method [1]. This enables us to control the errors in the material laws, conservations laws and compatibility conditions in contrast to the classical approach in which one may produce high numerical precision using FEM with material laws of far less accuracy. The data-driven problem can be expressed as an optimization problem: Find the set of points in the collection of material data points that minimizes the errors in the conservation laws, compatibility conditions and essential constraints [1,2].

The present contribution discusses a variational framework for the data-driven approach to computational mechanics suggested by Kirchdoerfer and Ortiz [1]. It introduces Lagrange multipliers for both the conservation laws and the compatibility condition in the continuous setting [3]. An interpretation of the resulting algorithm as a staggered scheme is also provided. From this generalization we obtain different Galerkin-based implementations. We provide several representative examples in order to justify the proposed variational formulation.

References

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5.11 Data mining in small-scale plasticity

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Dislocations are simplistic objects: they are one-dimensional, their motion is constrained by the crystallography and they are surrounded by a stress field that decays with $1/r$. However, once dislocations start to interact with themselves or with other microstructures, their collective behavior becomes extremely complex. This – despite the apparent simplicity of the individual object – is still far from completely being understood. While today powerful microscopy and simulation methods reveal many important information about systems of dislocations, the analysis of such data or even the comparison among different methods is still lagging behind. Systematic data mining is still far beyond the possibilities of today's methodologies. I will present a new unifying multiscale approach for characterizing and data mining of dislocation microstructures that works both for experiments and simulations and for very different length scales.

5.12 Data-assisted surrogate modeling of nonlinear solids

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Motivation. Aiming at drastic increases of efficiency for the solution of two-scale homogenization problems, we propose to a dedicated interpolation scheme coupled with a specialized sampling strategy.

Current state. In order to interpolate the *(pseudo-)hyperelastic material* law **[1]**

$$\boldsymbol{\varepsilon} \mapsto W(\boldsymbol{\varepsilon})$$

efficiently on training data $\left(\boldsymbol{\varepsilon}_i, W(\boldsymbol{\varepsilon}_i), \frac{\partial W}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}_i)\right)$, $i = 1, \ldots, p$, we split the strain as

$$\boldsymbol{\varepsilon} = \varepsilon \boldsymbol{N}^{\varepsilon}, \quad \varepsilon = \|\boldsymbol{\varepsilon}\|, \quad \boldsymbol{N}^{\varepsilon} = \frac{\boldsymbol{\varepsilon}}{\varepsilon}.$$

Then, the interpolation treats the training amplitudes ε_i and the training directions $\boldsymbol{N}^{\varepsilon_i}$ separately. For the latter, spherical basis functions (SBF) **[2]** are employed, linking this topic to the general field of scattered data interpolation on spheres. In the case of surrogate models for homogenized responses, the resulting evaluation is independent of the microstructure and reduces to few non-iterative function evaluations.

Sampling the direction space in a "uniform" manner, cf. Figure 1, comes along with advantages for

- offline costs (sampling, SBF parameter identification)
- resolution of the (unknown) anisotropy
- robustness.

Outlook. We discuss possible extensions to *problems of finite strain* and to *viscoelasticity*. There, additional constraints of the sampling space and path-dependency, respectively, pose new challenges.

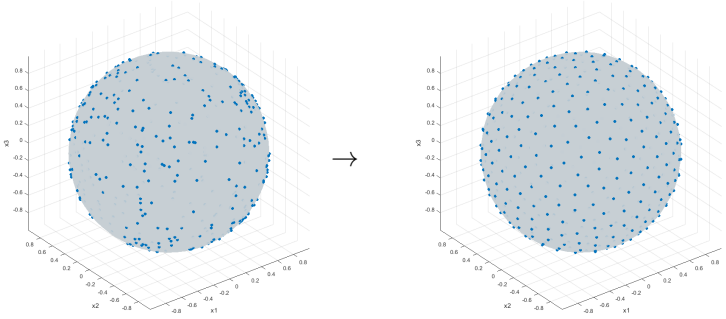

Figure 1: numerical procedure for uniform distributions of directions in $\mathbb{R}^3$

References

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[2] F. J. Narcowich, X.P. Sun, J. D. Ward, H. Wendland [2007]: "Direct and inverse Sobolev error estimates for scattered data interpolation via spherical basis functions", Foundations of Computational Mathematics **7**, 369–390

6 Venues and Locations

- Leuphana University of Lüneburg
  Universitätsallee 1, C 40.704 (Central Building)
  21335 Lüneburg
  How to reach Leuphana University of Lüneburg
  www.leuphana.de/en/services/travel-directions
- Helmholtz-Zentrum Geesthacht
  Max-Planck-Straße 1 (Nobel Pavillon) – start will be at building 31
  21502 Geesthacht
  How to reach Helmholtz-Zentrum Geesthacht
  https://www.hzg.de/about_us/visit_us/lageplan/geesthacht/index.php.en

7 Organizers

- Prof Dr.-Ing. Benjamin Klusemann
  Institute of Product and Process Innovation, Leuphana University of Lüneburg
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  https://www.leuphana.de/institute/ppi.html
  https://www.hzg.de/institutes_platforms/materials_research/materials_mechanics/joining_and_assessment/index.php.de
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