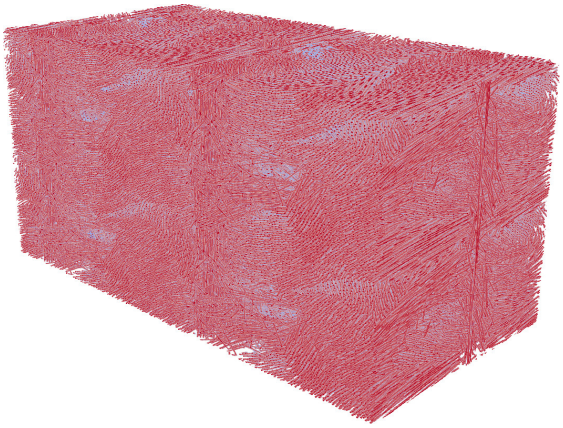
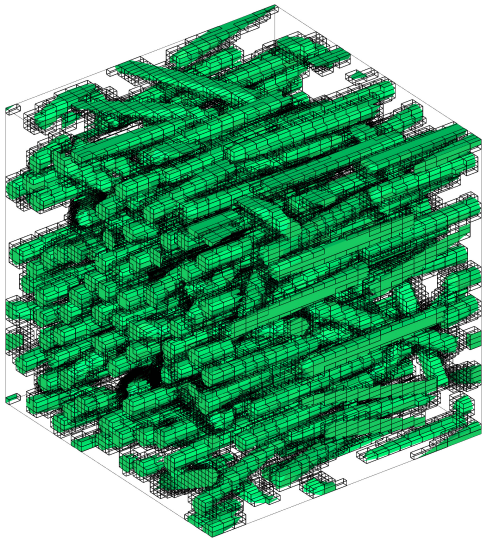
9th GAMM AG Data Workshop

University of Stuttgart
March 20/21, 2023





GAMM Activity Group on Data-driven Modeling and Numerical Simulation for Microstructured Materials

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Local organization
Prof. Tim Ricken and team
Institute of Structural Mechanics and Dynamics in Aerospace Engineering
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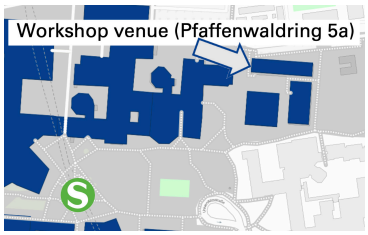
Contents

1 Practical information

1.1 Location

The workshop will take place in Pfaffenwaldring 5a on the campus in 70569 Vaihingen. It can be reached by **S1, S2, S3** from either Stuttgart central station as well as the airport (use exit "Universität"). From the S-Bahn stop, please follow the provided sketch to gain the SimTech building (Pfaffenwaldring 5a). The workshop takes place on the ground floor in **room 0.009**.



1.2 Welcome snack

We invite all participants to join us for a welcome snack at La Bruschetta on Monday from around 11:45. We will meet at the venue beforehand and walk to the restaurant (around 5 min. walk). In case you want to join us immediately "sur place", the address is Pfaffenwaldring 62, 70569.

1.3 Workshop dinner

The workshop dinner will take place in **Carls Brauhaus**, Stauffenbergstraße 1, 70173 Stuttgart. We will meet there around 18:30 (or you join us on the S-Bahn to get there after the discussion of the first day of the workshop).

1.4 Wifi access

Wireless network access is granted via `eduroam`.

2 Scientific Program

	Monday, March 20, 2023
11:45–12:50	**welcome lunch**
12:50–13:00	**opening**
13:00–13:25	**Sanath Keshav** Composite Boxels with imperfect Interfaces (ComBI) with FFT-based solvers
13:25–13:50	**Fadi Aldakheel** A combined EBSD and machine learning approach for efficient multi-scale modeling
13:50–14:15	**Mohammad Shojaee** Multiscale study of functionally graded shell lattice structures using physics guided neural networks
14:15–14:40	**Siva Teja Sala** Prediction and modification of deformation in thin Ti6Al4V sheets using artificial neural networks
14:40–15:05	**Frederic Bock** Data-driven and physics-based modelling for friction surfacing to identify and utilize process-structure relations under different environmental conditions
15:05–15:30	**coffee break**
15:30–15:55	**Lena Dyckhoff** Data-Driven Modeling of Yield Surfaces of Nanoporous Metals in Multiaxial Stress Space
15:55–16:20	**Balduin Katzer** Applying a query language to a graph database for detecting hidden propertiesin dislocation based plasticity
16:20–16:45	**Markus Kästner** Exploring structure-property linkages using descriptor-based microstructure reconstruction
16:45–17:10	**Alexander Hartmaier** Data-oriented constitutive models for polycrystalline metals
17:10–17:30	**discussion**
18:30–?	**workshop dinner**

	Tuesday, March 21, 2023
09:00–09:25	**Karl Kalina** Physics-augmented neural networks meet hyperelasticity
09:25–09:50	**Fabian Roth** Parametrised polyconvex hyperelasticity with neural networks
09:50–10:15	**Dominik Klein** Nonlinear electro-elastic finite element analysis with physics-augmented neural network constitutive models
10:15–10:40	**coffee break**
10:40–11:05	**Kevin Linka** Constitutive Artificial Neural Networks (CANNs) with applications to soft biological tissues
10:40–11:30	**Patrick Weber** Energy conservation for ANN material models: Comparing a weak enforcement with the penalty method to a strong enforcement utilizing a specific data loss function
11:30–11:55	**Julien Stöcker** Neural network based computational homogenization of arbitrary heterogeneous elastic mesostructures
11:55–12:20	**Julian Lißner** Double U-Net: Microstructure modeling via convolutional neural networks
12:20–12:30	**closing**
12:30–13:30	**farewell snack**

3 Participants

Local organizers

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3.1 Composite Boxels with imperfect Interfaces (ComBI) with FFT-based solvers

Sanath Keshav[1], Felix Fritzen[1], Matthias Kabel[2]

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Cohesive zones were first introduced to simulate the production of cracks caused by interfacial damage. However, the term is often used in a broader sense to refer to imperfect interfaces governed by constitutive traction separation laws. In unstructured finite element simulations, cohesive zones are discretized by specific interface conforming cohesive elements. The discretization of FFT-based methods is generally non-conforming to the interfaces; hence the classical interface cohesive elements cannot be employed. In this work, we propose a framework that is a generalization of composite boxels [Keshav, S. Fritzen, F. Kabel, M. 2022, Kabel, M et al. 2015] for interfacial damage modeling in FFT-based solvers. The special focus is on gathering the interface metadata from images using a novel image-based algorithm. An efficient implementation with a particular emphasis on numerical robustness is proposed. Numerical examples along with traction and stress field statistics comparing the proposed framework with unstructured finite element simulations are presented.

References

[1] Keshav, S., Fritzen, F., Kabel, M. [2023]: " FFT-based homogenization at finite strains using composite boxels (ComBo)", Journal of Computational Mechanics **71**, 191–212

[2] M. Kabel, D. Merkert, M. Schneider [2015]: " Use of composite voxels in FFT-based homogenization", Computer Methods in Applied Mechanics and Engineering **294**, 168–188

[3] M. Leuschner, F. Fritzen [2018]: "Fourier-accelerated Nodal Solvers (FANS) for homogenization problems", Journal of Computational Mechanics **62,3**, 359–392

3.2 A combined EBSD and machine learning approach for efficient multi-scale modeling

F. Aldakheel

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Computational material modeling using advanced numerical techniques speeds up the design process and reduces the costs of developing new products. In the field of multiscale modeling, huge computation costs are expected for modeling heterogeneous materials while trying to reach high accuracy levels. In this work, a machine learning approach, namely the Convolutional Neural Network (CNN), is developed as a solution providing a high level of accuracy, while being computationally efficient.

The data set for training and testing the CNNs consists of images of real microstructures (input) and the homogenized stiffness components of the RVE (output). So far, research in this area has mainly focused on two-phase microstructures with isotropic components. Imaging techniques such as Electron Backscatter Diffraction (EBSD), allow the visualization of complex crystalline structures, with their orientation in space, and motivate an extension of these CNNs to more complex microstructures.

In this work, a machine learning approach is proposed for anisotropic crystalline RVEs randomly oriented in space. Hereby, the 21 independent components of the stiffness matrix are predicted. Furthermore, the applicability of *data augmentation* in this talk will be discussed. The model efficiency is demonstrated by the means of some representative examples.

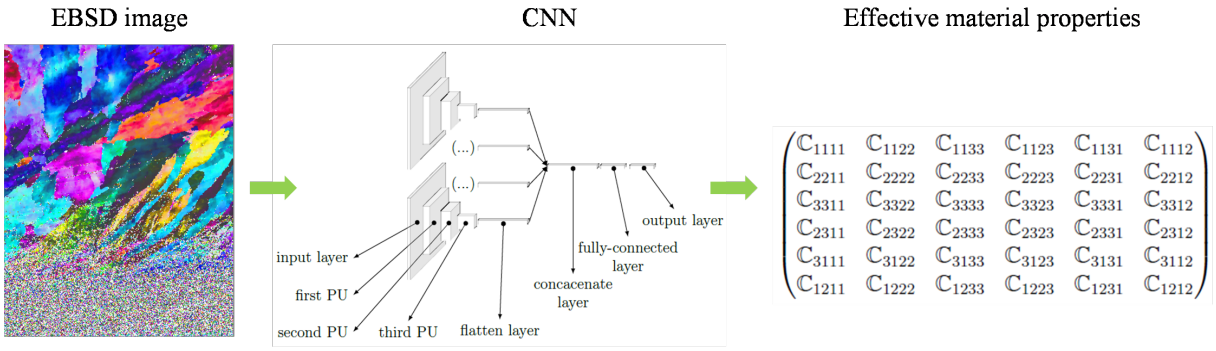

Figure 1: EBSD and CNN for fast prediction of effective material properties.

References

[1] F. Aldakheel, C. Soyarslan, H. S. Palanisamy, E. S. Elsayed [2023]: "Machine Learning Aided Multiscale Magnetostatics", arXiv preprint **arXiv:2301.12782**

3.3 Multiscale study of functionally graded shell lattice structures using physics-guided neural networks

M. Shojaee[1], I. Valizadeh[1], D.K. Klein[1], O. Weeger[1]

[1]: Cyber Physical Simulation, Technical University of Darmstadt, Germany; *mail:* weeger@cps.tu-darmstadt.de

Additive manufacturing techniques have allowed for the production of functionally graded lattices with customized mechanical properties. Among lattice geometries, triply periodic minimal surfaces (TPMS) are of particular interest due to their geometric and mechanical properties, making them applicable in various fields with efficient design. However, uncertainties remain regarding the mechanical behavior of shell lattices, including their stability, deformability, and response to external forces.

In this regard, a theoretical and experimental study on the nonlinear microscale mechanical behavior of the Schwarz primitive TPMS is conducted using physics-guided neural networks [1]. The study includes a systematic procedure that covers micro-scale to full-scale modeling and simulation. Specifically, the nonlinear microscale behavior of the parameterized Schwarz primitive through theoretical and experimental methods is investigated. The microstructure framework involves simulating representative volume elements (RVEs) with different repeat unit cells to evaluate the RVE convergence and the size dependency of the effective behavior. A parametric material model based on a physics-guided feed-forward neural network is employed to predict the constitutive model of graded elastic solid structures at any arbitrary material point. Furthermore, the linear static behavior of graded lattices made of Schwarz primitives is also examined on the macroscale level to confirm the reliability and efficiency of the method. Then they are demonstrated through the examination of homogeneous and graded lattice models on a macroscale level. Three different models are used: a full-scale model, a homogenized finite element model using Abaqus, and a linear 3D elastic theory using the differential quadrature method.

Finally, the convergence and accuracy of these methods for the static mechanical behavior at the finite deformation continuum level are discussed. In conclusion, this study provides valuable insights into the nonlinear microscale mechanical behavior of TPMS and the linear static behavior of graded lattices made of Schwarz primitives on a macroscale level. The proposed multiscale approach is expected to enhance the understanding of the mechanical behavior of functionally graded lattice structures and support their design and fabrication for a wide range of applications.

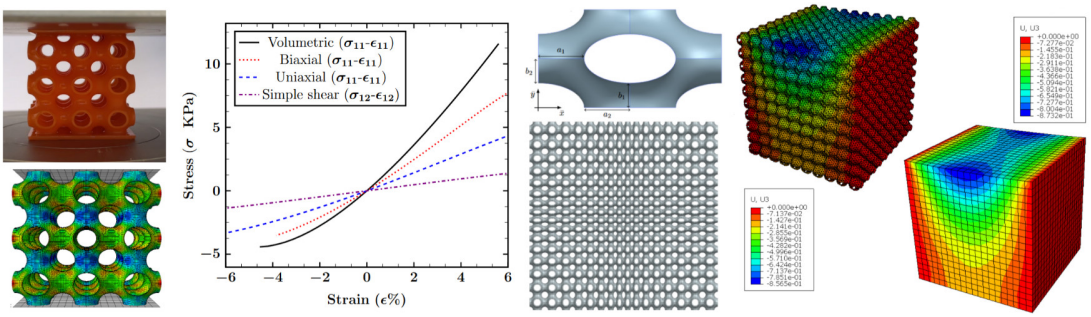

Figure 1: Illustration of the multiscale simulation framework for functionally graded shell lattice structures

References

[1] M. Shojaee, I. Valizadeh, D.K. Klein, P. Sharifi, O. Weeger [2023]: "Multiscale simulation of additively manufactured shell lattice metamaterials with physics-guided neural networks", to be submitted

3.4 Prediction and modification of deformation in thin Ti6Al4V sheets using artificial neural networks

S. T. Sala[1], F. E. Bock[1], D. Pöltl[2], B. Klusemann[1,2], N. Huber[1,3], N. Kashaev[1]

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[3]: Institute of Materials Physics and Technology, Hamburg University of Technology, Eißendorfer Straße 42, 21073 Hamburg, Germany.

The accurate bending of sheet metal structures is critical in a variety of industrial and scientific contexts, whether it is to modify existing components or achieve specific shapes. Laser peen forming (LPF) (see Fig. 2) is an advanced process for sheet metal applications that involves using mechanical shock waves to deform a specific area to a desired radius of curvature. The degree of deformation achieved through LPF is affected by various experimental factors such as laser energy, the number of peening sequences, and specimen thickness. Therefore, it is important to understand the complex dependencies and select the appropriate LPF process parameters for forming or correction purposes. This study aims to develop a data-driven approach to predict the deformation obtained from LPF for different process parameters. The experimental data is used to train, validate, and test an artificial neural network (ANN). The trained ANN successfully predicted the deformation obtained from LPF. A innovative process planning approach is developed to demonstrate the usability of ANN predictions in achieving the desired deformation in a treated area. The effectiveness of this approach is demonstrated on three benchmark cases involving thin Ti-6Al-4V sheets: deformation in one direction, bi-directional deformation, and modification of an existing deformation in pre-bent specimens via LPF.

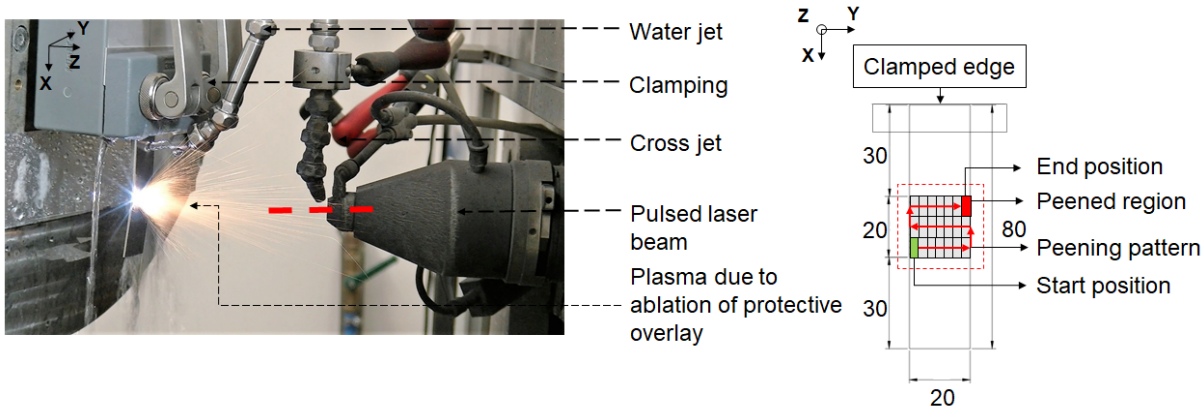

Figure 2: Experimental setup of LPF process where the LPF specimen is covered with a sacrificial overlay and with a laminar flow of water as a transparent overlay. One edge of the specimen is clamped and the specimen moves relative to the laser beam generating, a zig-zag peening pattern.

3.5 Data-driven and physics-based modelling for friction surfacing to identify and utilize process-structure relations under different environmental conditions

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In the last decade, there has been a surge in successful applications of machine learning models serving as a key to unlock relationships along the process-structure-property-performance chain for vastly different problems within the fields of materials mechanics. The consideration of physical laws in data-driven modelling has recently been shown to enable enhanced prediction performances and increased generalization while required amounts of data can be reduced, in comparison to solely using either one of these modelling approaches.

In this presentation, a simulation-assisted machine-learning (ML) framework is discussed on the example of friction surfacing, a solid-state layer deposition process that can be used for repair or coating applications. The aim is to use ML methods to foresee and understand the influence of process parameters and environmental conditions on resulting deposit geometry and process behavior. Special attention is given to influences of the maximum temperature on prediction targets during the process provided by a numerical heat transfer model. To exploit the diverse potential of different ML algorithms and select the best for the particular problem and available data, various machine-learning algorithms are evaluated. In addition, feature dependencies of predicted targets are identified. For the generation of an experimental data set with as few samples as possible, two separate designs of experiments are conducted, one for variation of process parameters as well as another for the variation of substrate and backing material properties. The aim is to also represent the cross parameter space between both individual spaces, which was achieved and enabled a reduction of experiments by approximately 45 % in comparison to performing a similar design of experiments that comprises both subspaces.

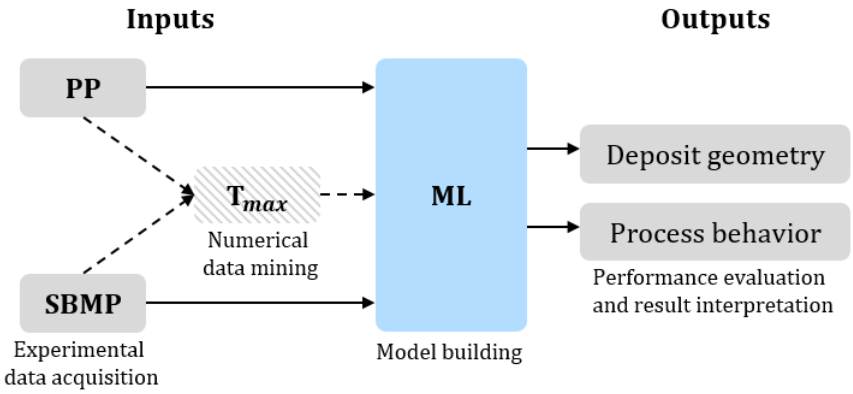

Figure 3: Schematic of the data workflow, originating from either process parameter space (PP) or substrate and backing material property space (SBMP), including or excluding the numerically determined maximum temperature T_{max} to be processed by machine learning regression to predict the targets: process deposit geometry and process behavior, respectively.

3.6 Data-Driven Modeling of Yield Surfaces of Nanoporous Metals in Multiaxial Stress Space

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Nanoporous metals, built out of complex ligament networks, can be produced with an additional level of hierarchy [1]. The resulting complexity of the structure makes modeling of the mechanical behaviour computationally highly expensive and time consuming. In addition, multiaxial stresses occur in the higher hierarchy ligaments. Therefore, knowledge of the multiaxial material behaviour, including the 6D yield surface, is required. For finite element (FE) modeling, we separate the hierar-chical nanoporous structure into the upper and lower level of hierarchy. This allows independent adjustment of structural parameters on both hierarchy levels and therefore an efficient analysis of structure-property-relationships. Furthermore, a promising approach to significantly reduce com-putational cost is to use surrogate models and FE-beam models to predict the mechanical behav-iour of the lower level of hierarchy. As a first step towards such a model, we studied the elastic behaviour and yield surfaces of ideal-ized diamond and Kelvin beam models using FE simulations. The yield surfaces exhibit pronounced anisotropy, which could not be described properly by models like the Deshpande-Fleck model for isotropic solid foams [1]. For this reason, we used data-driven and hybrid artificial neural networks, as well as data-driven support vector machines and compared them regarding their potential for the prediction of these yield surfaces. All considered methods turned out to be well suited and resulted in relative errors < 4.5. Of the considered methods, support vector machines exhibit the highest generalization and accuracy in 6D stress space and outside the range of the used training data.

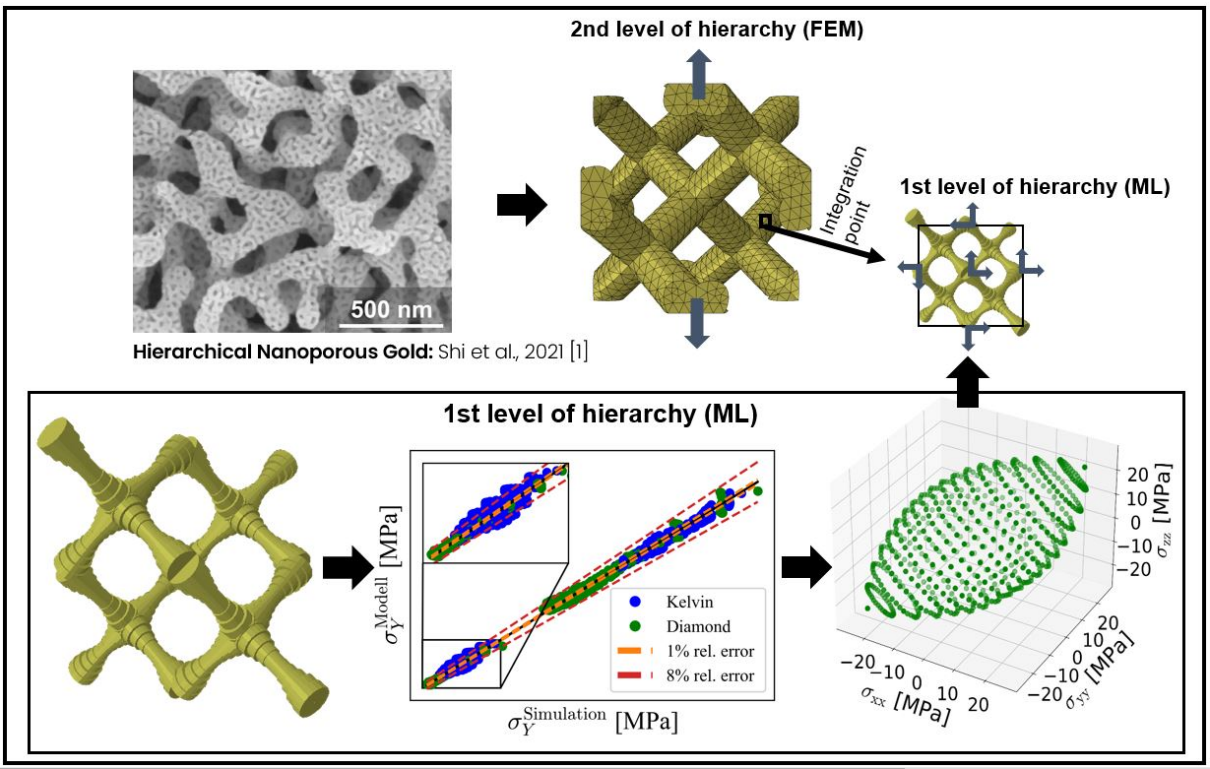

Figure 1: Schematic of the workflow to integrate data-driven prediction of yield surfaces by machine learning algorithms into hierarchical FE modeling of nanoporous metals.

References

[1] S. Shi et al. [2021]: "Scaling behavior of stiffness and strength of hierarchical network nanomaterials", Science **371**, 1026-1033

3.7 Applying a query language to a graph database for detecting hidden propertiesin dislocation based plasticity

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Graph analytics has been an emerging form of data analysis in the recent years. The method is usually appliedto understand complex relationships between linked entitiy data in a network, e.g. shortest path solution,finding connected components or predicting missing links. Graphs are mathematical structures used to modeldifferent types of relationships. In this contribution we use graph analysis to detect hidden properties indislocation based plasticity. We set a graph database with the management system "Neo4J", connecting themicrostructure data in a graph structure. This leads to the possibility to query within the microstructure graphdata with the query language "Cypher". We create a method to systematically extract physical informationabout the investigated material microstructures. This enables the extraction of features in a way that yield anew approach for homogenization based on physical mechanisms.

We demonstrate the application of the graph database query language as well as extracted features of dislocationnetworks, which pave the way to a more naturally handling of complex data. We compare the analysismethod and results from the graph databases with results from relational database analysis [1,2]. Finally, wegive an outlook in several procedures, which are naturally applicable to the graph database, like the creationof hyper graphs for slimming the data, graph property predictions or the application of graph neural networksfor the prediction of future graph states.

References

[1] B. Katzer, K. Zoller, D. Weygand, K. Schulz. [2022]: "Identification of dislocation reaction kinetics in complex dislocation networks for continuum modeling using data-driven methods", Journal of the Mechanics and Physics of Solids, 105042

[2] B. Katzer, K. Zoller, J. Bermuth, D. Weygand, K. Schulz. [2023]: "Characterization of Lomer junctions based on the Lomer arm length distribution in dislocation networks", Scripta Materialia 226, 115232

3.8 Exploring structure-property linkages using descriptor-based microstructure reconstruction

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Establishing and inverting structure-property-linkages is a central topic in inverse computational materials engineering and offers great potential for acceleration by data-driven techniques. For this purpose a microstructure reconstruction approach is presented and used in an automatic exploration and inversion framework.

Recently developed algorithms allow for generating RVEs of complex microstructures given a set of microstructure descriptors [1, 2]. The central idea is to formulate microstructure reconstruction as a differentiable optimization problem, allowing for highly efficient gradient-based quasi-Newton optimizers. The approach is implemented in MCRpy [3] and an extension by a suitable post-processing as well as a validation are presented in [4]. An overview over this method is given and current extensions are highlighted.

A promising application of descriptor-based reconstruction lies in the exploration and inversion of structure-property linkages. For this purpose, a large data set of structure-property pairs is needed due to the complex and nonlinear nature of the underlying relation. Therefore, computational augmentation promises to allow for data-driven approaches even on the basis of a small data set. For this purpose, microstructure images in the data-base are characterized by translation-invariant descriptors by MCRpy [3]. Then, three-dimensional microstructures are reconstructed from the descriptors and the effective properties are determined by numerical simulations. Finally, all descriptor-property pairs in the data base are used to predict potentially improved microstructures in terms of their associated descriptors. These descriptors can be passed to the reconstruction and simulation tools to repeat the same process in an automated data-driven materials design loop.

References

[1] P. Seibert, M. Ambati, A. Raßloff, M. Kästner [2021]: Reconstructing random heterogeneous media through differentiable optimization, Computational Materials Science

[2] P. Seibert, A. Raßloff, M. Ambati, M. Kästner [2022]: Descriptor-based reconstruction of three-dimensional microstructures through gradient-based optimization, Acta Materialia

[3] P. Seibert, A. Raßloff, K. Kalina, M. Ambati, M. Kästner [2022]: Microstructure Characterization and Reconstruction in Python: MCRpy, Integrating Materials and Manufacturing Innovation

[4] P. Seibert, A. Raßloff, K. Kalina, J. Gussone, K. Bugelnig, M. Diehl, M. Kästner [2023]: Two-stage 2D-to-3D reconstruction of realistic microstructures: Implementation and numerical validation by effective properties (submitted)

3.9 Data-oriented constitutive models for polycrystalline metals

R. Shoghi[1], J. Schmidt[1], A. Hartmaier[1]

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In classical constitutive modeling, the response of a material to mechanical loads is described by explicit mathematical expressions for the relations between stress and strain or strain-rates. Such mathematical formulations can become rather intricate, e.g., when describing history-dependent plasticity on the level of single-crystalline regions, as it is done in crystal plasticity. Yet, typically, such closed-form constitutive models do not take into account microstructural features, as grain size and shape or the crystallographic texture. This situation is rather unsatisfactory from a materials science point-of-view, as it is known that such microstructural features do not only control the mechanical behavior of a material but, moreover, they can be subject to change during plastic deformation. In this work, two approaches are highlighted how microstructure-sensitive data on plastic deformation of polycrystals are used to train numerically efficient machine learning models as constitutive relations that can directly be applied in finite-element models of engineering structures.

In the first approach, the anisotropic yield function Barlat Yld2004-18p is parametrized from micromechanical simulations for different textures. The structure-property relationship between the crystallographic texture and the material parameters is then identified by applying supervised Machine Learning (ML) methods on that data set. As part of this identification process, different descriptors for the crystallographic texture are tested in their capability to relate unimodal and also fibre textures to a unique set of anisotropic parameters.

In the second approach, it is investigated how an optimal data-generation strategy for the training of a ML model can be established that produces reliable and accurate ML yield functions with the least possible effort. It is shown that even for materials with a significant plastic anisotropy, as polycrystals with a pronounced Goss texture, 300 data points representing the yield locus of the material in stress space, are sufficient to train the ML yield function successfully. Furthermore, the formulation of a full ML flow rule is discussed, including strain hardening captured from micromechanical data.

References

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3.10 Physics-augmented neural networks meet hyperelasticity

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Within this contribution, we present a hyperelastic constitutive model based on physics-augmented neural networks (PANNs) which fulfills all common physical requirements on this model class by construction and, in particular, is applicable for compressible material behavior [1]. The model combines the theory of hyperelasticity developed in the last decades with the up-to-date techniques of machine learning, by formulating a hyperelastic potential as an input-convex neural network (ICNN). This potential fulfills conditions such as compatibility with the balance of angular momentum, objectivity, material symmetry, polyconvexity, and thermodynamic consistency. Analytical growth terms and normalization terms, formulated for both isotropic and transversely isotropic material behavior, are used to ensure a physically sensible stress behavior of the model and to guarantee that the undeformed state is stress free and with zero energy. The non-negativity of the hyperelastic potential is numerically verified by sampling the space of admissible deformations states. The applicability of the model is demonstrated by calibrating it on data generated with a neo-Hooke potential. Furthermore, its extrapolation capability is compared to models with reduced physical background, showing excellent and physically meaningful predictions with the proposed PANN approach, see the Finite Element simulations given in Figure 1. Finally, the application of NNs enriched with a well-founded physical background is shown in the data-driven multiscale scheme FE$^{\text{ANN}}$ [2].

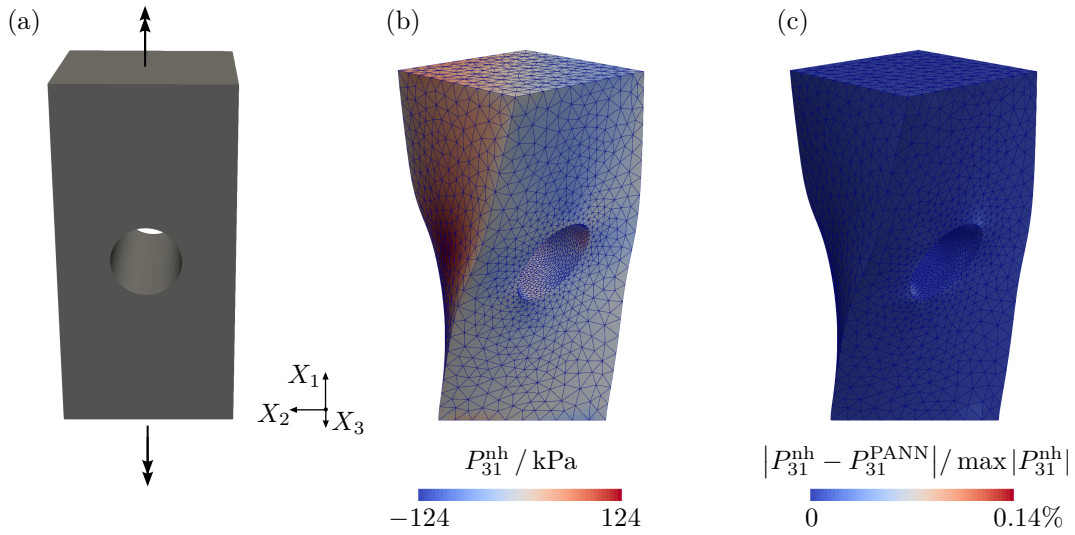

Figure 1: Finite Element simulation of a torsional sample: (a) loading conditions, (b) stress field P_{31}^{nh} calculated with a neo-Hooke model by specifying a distortion of $\hat{\phi} = 45°$, and (c) relative error of the stress field P_{31}^{PANN} predicted with the PANN. The model was trained with only uniaxial stress-strain data and contains only 4 neurons in one hidden layer [1].

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3.11 Parametrised polyconvex hyperelasticity with neural networks

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Convexity is a convenient property of mathematical functions in many applications. In the framework of hyperelastic constitutive modeling, the polyconvexity condition is widely used as it implies ellipticity and thus ensures well-behaving numerics [1]. On the other side, assuming convexity constrains the function space a model can represent. While for some applications, this constraint is well motivated, it is too restrictive for other use cases. And, finally, there are applications where a function can be motivated to be convex in some of its arguments, while it should not necessarily be convex in its other arguments.

In this work [2], partially input-convex neural network (pICNN) architectures are applied for the modeling of parametrised polyconvex hyperelastic potentials. Receiving two different sets of input arguments, pICNNs are convex in one of them, while for the other they represent arbitrary relationships which are not necessarily convex. Three different pICNN architectures are investigated, which are all based on feed-forward neural networks. Extending the work of [3], the proposed model fulfills all common constitutive conditions of hyperelasticity by construction. The applicability of the model is demonstrated by calibrating it on data generated with an analytical parametrized potential.

Combining a sound mechanical basis with the extraordinary flexibility that neural networks offer, the model will be able to represent the behavior of materials with parametrized microstructures, allowing for efficient multiscale simulations and optimization of microstructures. Furthermore, the extension towards multi-physical behavior is straightforward.

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3.12 Nonlinear electro-elastic finite element analysis with physics-augmented neural network constitutive models

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In the last decades, a vast amount of highly specialized metamaterials has been developed and, with advancing requirements in engineering applications, the trend is growing. Often comprised of complex multiphysical microstructures, these materials can be tailored for each specific application. At the same time, this sets a challenge for the mechanical description of such materials, as they behave highly nonlinear. Thus, we envision the use of physics-augmented neural networks, circumventing the current limitations of analytically formulated material models.

In [2], the concept of polyconvex hyperelastic neural network constitutive models [1] was extended towards electro-mechanically coupled material behavior at finite deformations. Using electro-mechanically coupled invariants as inputs for convex neural networks, a polyconvex internal energy is constructed. In this way, the model fulfills common constitutive conditions such as objectivity and ellipticity by construction. Augmenting the neural network with constitutive conditions is not only important to arrive at reliable, i.e., physically sensible model predictions. More than that, it allows for model calibration with small datasets, which are usually only available in engineering applications, e.g., from experimental material characterization tests.

Finally, the model is applied for the finite-element analysis of microstructured electro-active materials [3]. In this way, it is demonstrated how highly flexible neural network constitutive models can be applied for efficient multiscale simulations. Furthermore, the straightforward applicability of the neural network constitutive model in a finite element framework is shown.

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3.13 Constitutive Artificial Neural Networks (CANNs) with applications to soft biological tissues

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The classical, theory-driven approach to describe the deformation of a material body relies on the formulation of constitutive equations relating strains and stresses. A drawback of this approach are the efforts typically required to develop appropriate functional relations and identify material parameters .

These efforts are not required in data-driven approaches to constitutive modeling. To combine the advantages and overcome the disadvantages of both theory- and data-driven constitutive modeling, we have developed the novel concept of Constitutive Artificial Neural Networks (CANNs). This machine learning approach to data-driven constitutive modeling does not require any major a priori assumptions about the constitutive law but yet incorporates substantial theoretical knowledge about continuum mechanics and constitutive theory. This way, CANNs are able to learn the constitutive law of a material from relatively small amounts of stress-strain data. Moreover, by their ability to incorporate also non-mechanical data, they cannot only describe the constitutive behavior of known materials but also predict the one of new materials, making them the ideal tool for computational biomechanics. Using data from mechanical tests, histological analyses and advanced imaging, this architecture is trained to predict the nonlinear macroscopic mechanical properties of e.g. arterial and brain tissue.

Moreover, we demonstrate that our machine learning architecture is not limited to predictions but can also help to understand the mechanics of soft tissue. Using concepts of explainable artificial intelligence, we demonstrate that it enables the automatic, systematic and largely unbiased quantification of the importance of different microstructural features for the macroscopic mechanical properties.

3.14 Energy conservation for ANN material models: Comparing a weak enforcement with the penalty method to a strong enforcement utilizing a specific data loss function

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In phenomenological material modeling, macroscopic constitutive equations are based on experimental observations and properly defined physical laws. For more than thirty years, these classical methods are accompanied by data-based approaches in order to circumvent the traditional definition of analytical material functions and the subsequent fitting of their material parameters. In this contribution, we follow the method of training a feedforward artificial neural network (ANN) as constitutive model, directly from given strain and stress data.

A major drawback of this and other data-based methods is the fact, that the corresponding material models lack physical properties. Such algorithms have to learn them implicitly from the given data. This problem becomes worse if only a small amount of data is available. Therefore, current developments in ANN material modeling aim for the incorporation of physical laws. For example, in Weber et al. [1], constrained optimization techniques are used to enforce physical constraints, e.g. energy conservation, weakly during the training process. In Klein et al. [2], input convex neural networks are used to approximate hyperelastic material behavior. The specific ANN definition enforces energy conservation in a strong sense, but needs additional derivatives of the ANN output. An overview is given in Fig. 1.

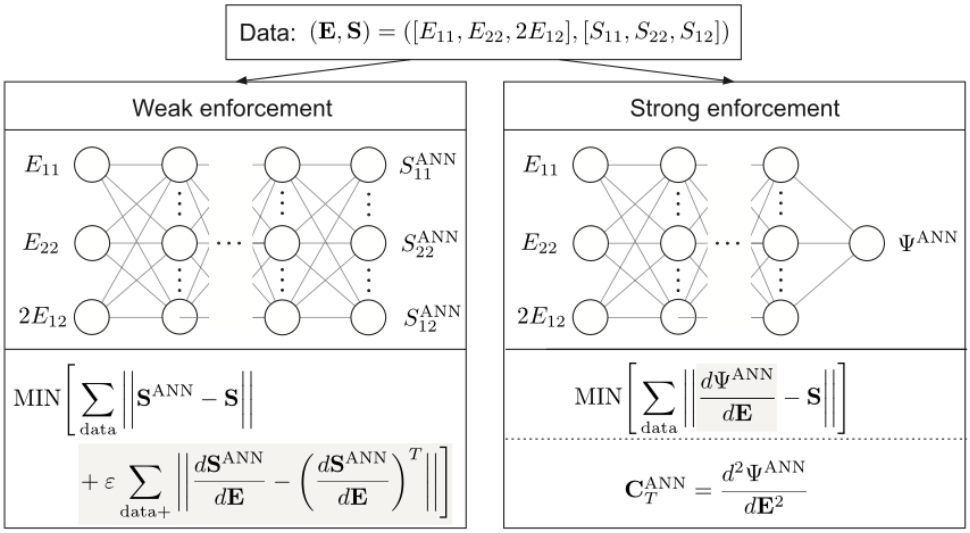

Figure 1: Comparison between weak enforcement of energy conservation via error term extension (left) and strong enforcement with a specific ANN output and stress definition (right)

In this contribution, we compare these two methods of enforcing energy conservation for ANN material modeling. Different sizes of synthetic data sets are gathered from an analytical hyperelastic material model at a plain stress state. With both approaches, corresponding ANN material models are generated. They are compared with respect to training time, training data error, their performance on unknown data on material level and their performance within finite element calculations of plain stress structures.

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3.15 Neural network based computational homogenization of arbitrary heterogeneous elastic mesostructures

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Direct numerical analysis of advanced composite materials with heterogeneous mesostructures by means of homogenization-based multiscale modeling poses a computationally expensive challenge in large-scale engineering applications. The required computational effort can be reduced by employing Machine Learning methods for computational homogenization. Typically, one unit cell with representative characteristics of the heterogeneous structure is numerically investigated for this method. This limitation to a singular representation presents a simplification of the real composition.

However, previous contributions have shown that Convolutional Neural Networks (CNN) exhibit high accuracy when utilized for homogenization of arbitrary heterogeneous structures employing Statistical Volume Elements (SVE) [1,2]. The SVE allow for the consideration of the naturally occurring fluctuations within the composite material.

This contribution investigates the applicability of the former findings to multiscale analysis. Therefore, differently constituted SVE and their respective constitutive response under arbitrary loading within the elastic regime are evaluated. Those are utilized to obtain a generalized Neural Network constitutive model which can be applied in Finite Element (FE) Analysis as a substitute for direct evaluation of the SVE within an FE^2 framework. Primarily, two different approaches for the consideration of the mesoscale composition are investigated. They are compared to a multiscale reference solution with respect to accuracy in the homogenization task and required computational effort. Within the first approach, a CNN is utilized to extract a one-dimensional representation from the mesostructure, while in the second approach, this is replaced by the Feed Forward Neural Network with scalar-valued volume fraction as an input. Both approaches employ the constitutive relation of the macroscopic strains together with the respective representation of arbitrary mesostructures to compute the macroscopic stresses.

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3.16 Double U-Net: Microstructure modeling via convolutional neural networks

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High performance materials are tuned by optimizing the material on its microscale. Manufacturing processes as well as the required tests during development lead to exorbitant costs and time investments. To improve the efficiency of the design loop, intermediate processes can be substituted by numerical simulations. Nevertheless, due to the representation of the microstructured material via (usually high resolution) images, direct simulations remain computationally costly [1]. One approach to reduce the computational cost is via machine learning.

In microstructure modeling, convolutional neural networks (Conv Nets) have recently gained popularity. One major advantage of Conv Nets is that they operate directly on the image data with no further information required for the prediction. The rise in popularity was amongst others due to the development of the so called *U-net* [2], which is a Conv Net layout designed for image predictions based on image inputs, well suited to predict the full field solution of a microstructured image, e.g. the thermal flux. If the data is available, the Conv Net can be expanded to predict any physical behaviour of the microstructured material.

Improvements of the U-net were found by an elaborate extension of the original design and the implementation of a multilevel optimization scheme. Our new model is applied to predict the thermal behaviour of the microstructured material for near arbitrary microstructure input, i.e. by allowing for highly variable microstructure characteristics, input resolutions as well different material phase contrasts, i.e. conducting as well as insulating inclusions.

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