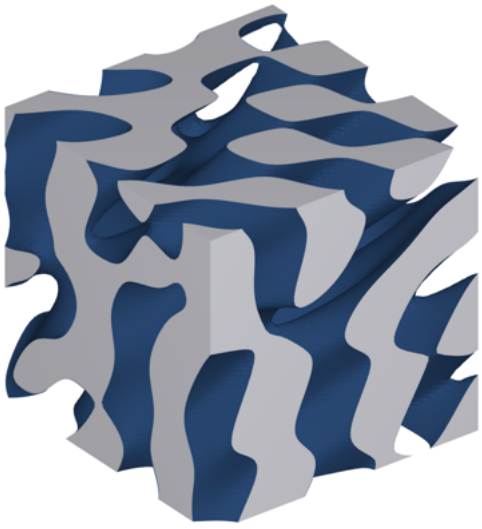
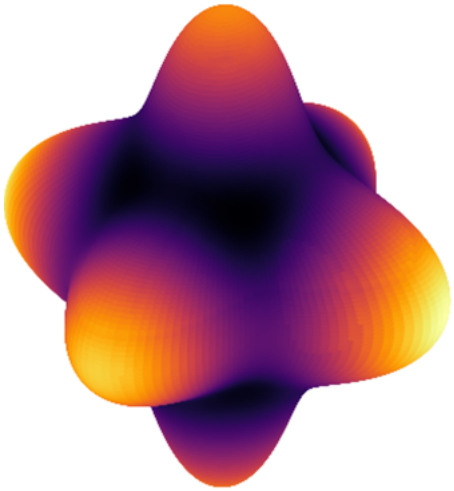
11th GAMM AG Data Workshop

TU Dresden
February 06/07, 2024





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

AG Data Chairs
Prof. Benjamin Klusemann · Leuphana University & Hereon · benjamin.klusemann@leuphana.de
Prof. Felix Fritzen · University of Stuttgart, Data Analytics in Engineering · fritzen@simtech.uni-stuttgart.de

Local organization
Dr. Karl Kalina · Institue of Solid Mechanics · TU Dresden
Prof. Markus Kästner and team · Institue of Solid Mechanics · TU Dresden

Contents

1 Practical information **4**

1.1 Location . . . 4
1.2 Welcome snack . . . 4
1.3 Workshop dinner . . . 4
1.4 Workshop lunch . . . 4
1.5 Wifi access . . . 4

2 Scientific Program **5**

3 Participants **7**

4 Abstracts **9**

4.1 *J. Schommartz, J. Alzate Cobo, D. Klein, O. Weeger:* A physics-enhanced, neural network based modeling approach for hyperelastic beams . . . 9
4.2 *L. Linden, K. A. Kalina, J. Brummund, M. Kästner:* Automated constitutive modeling of hyperelastic solids based on physics-augmented neural networks . . . 10
4.3 *M. Körbel, D. K. Klein, O. Weeger:* Stochastic hyperelastic constitutive modeling with Bayesian neural networks . . . 11
4.4 *D. K. Klein et al.:* Neural networks meet hyperelasticity: On limits of polyconvexity . . . 12
4.5 *A. Raßloff, P. Seibert, K.A. Kalina, M. Kästner:* Inverse design of spinodoids from sparse data through Bayesian optimization . . . 13
4.6 *P. Seibert, A. Raßloff, K. Kalina, M. Kästner:* Recent progress and challenges in descriptor-based microstructure reconstruction . . . 14
4.7 *L. Scholz, F. Fritzen:* Influence of grain boundaries on the overall diffusivity in polycrystalline solids . . . 15
4.8 *Melching et al.:* Advanced fracture mechanical analysis using digital image correlation, explainable machine learning, and data science . . . 16
4.9 *C. Haag, M.-A. Keip and F. Fritzen:* Knowledge-constrained splines for the prediction of physical phenomena . . . 17
4.10 *J. Schmidt, A. Hartmaier:* A Texture-Dependent Yield Criterion . . . 18
4.11 *F. Fritzen, J. Herb, S. Sharba:* Parameterized Nonuniform Transformation Field Anaylsis . . . 19
4.12 *G. Hütter, N. Lange, B. Kiefer:* A monolithic hyperintegrated ROM FE^2 method with clustered training strategy . . . 20
4.13 *I. Plyushchay, Z. Wei, S. Gemming:* Ab initio modeling of solid solution softening and hardening effects in Al-Mg-Zr-Si aluminum alloys and aluminum wrought alloys. . . . 21
4.14 *L. Dyckhoff, N. Huber:* Toward Hierarchical Modeling: Machine Learning for Describing Elastic-Plastic Behavior in Nanoporous Metals . . . 22
4.15 *Kian P. Abdolazizi, Kevin Linka, Christian J. Cyron:* Viscoelastic Constitutive Artificial Neural Networks (vCANNs) – a framework for data-driven anisotropic nonlinear finite viscoelasticity . . . 23
4.16 *R. Shoghi, L. Morand, D. Helm, A. Hartmaier:* Optimizing Machine Learning Yield Functions Using Active Learning for Support Vector Classification . . . 24
4.17 *M. Harnisch, T. Bartel, B. Schweizer, A. Menzel:* Enhancing data-driven inelasticity with neural networks: Opportunities in computational mechanics . . . 25
4.18 *K. A. Meyer, F. Ekre, R. Jänicke:* Thermodynamically consistent neural network plasticity modeling and discovery of evolution laws . . . 26

4.19 *M. Abendroth, A. Malik, G. Hütter, B. Kiefer:* A Hybrid Approach to Model the 3D Inelastic Deformation Behavior of Cellular Media Using Neural Networks 27

4.20 *K. A. Kalina et al.:* Physics-augmented neural networks for constitutive modeling of elasticity and viscoelasticity 28

1 Practical information

1.1 Location

The workshop will take place in **Andreas-Pfitzmann-Bau (APB), Room APB E023**, Nöthnitzer Str. 46, 01187 Dresden. It can be reached by tram **3, 8**. If you are traveling from the airport, we recommend taking the S-Bahn to the main train station and then continuing by tram.

1.2 Welcome snack

We invite all participants to join us for a welcome light lunch at the **Foyer of Andreas-Pfitzmann-Bau** on Tuesday from around 12:00. Registration for the workshop is possible from 11:00.

1.3 Workshop dinner

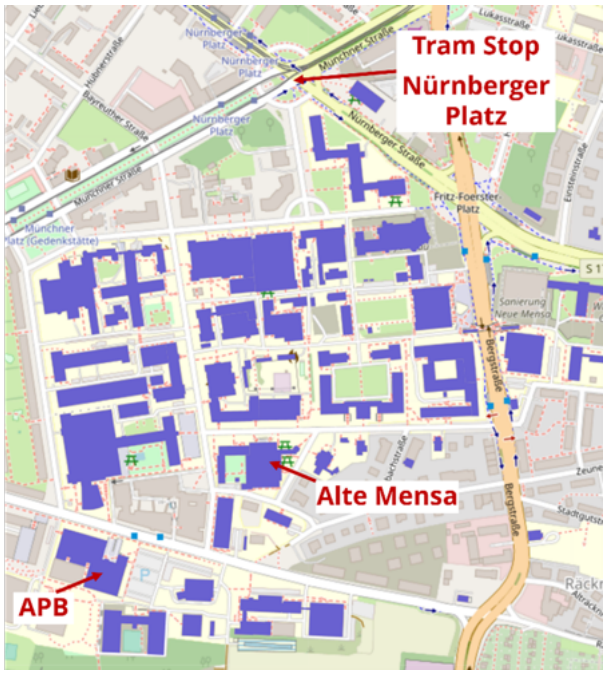
The workshop dinner will take place in the restaurant **Neue Sachlichkeit**, Kraftwerk Mitte 7, 01067 Dresden. We will meet there around 19:00 (or you join us on the tram/S-Bahn to get there after the discussion of the first day of the workshop).

1.4 Workshop lunch

On the second day of the workshop, a lunch will take place in the dining hall **Alte Mensa**, Momsenstraße 13, 01069 Dresden. You will receive a meal voucher when you register.

1.5 Wifi access

Wireless network access is granted via **eduroam**.



https://navigator.tu-dresden.de

www.google.de/maps

2 Scientific Program

	Tuesday, February 06, 2024
11:00–12:45	**Registration**
12:00–12:45	**Welcome lunch**
12:45–13:00	**Welcome adress**
13:00–13:25	**J. O. Schommartz** A physics-enhanced, neural network based modeling approach for hyperelastic beams
13:25–13:50	**L. Linden** Automated constitutive modeling of hyperelastic solids based on physics-augmented neural networks
13:50–14:15	**M. Körbel** Stochastic hyperelastic constitutive modeling with Bayesian neural networks
14:15–14:40	**D. K. Klein** Neural networks meet hyperelasticity: On limits of polyconvexity
14:40–15:05	**Coffee break**
15:00–15:25	**A. Raßloff** Inverse design of spinodoids from sparse data through Bayesian optimization
15:25–15:50	**P. Seibert** Recent progress and challenges in descriptor-based microstructure reconstruction
15:50–16:15	**L. Scholz** Influence of grain boundaries on the overall diffusivity in polycrystalline solids
16:15–16:40	**Coffee break**
16:40–17:05	**D. Melching** Advanced fracture mechanical analysis using digital image correlation, explainable machine learning, and data science
17:05–17:30	**C. Haag** Knowledge-constrained splines for the prediction of physical phenomena
17:30–17:55	**J. Schmidt** A Texture-Dependent Yield Criterion
19:00–?	**Workshop dinner**

	Wednesday, February 07, 2024
09:00–09:25	**F. Fritzen** Parameterized Nonuniform Transformation Field Anaylsis
09:25–09:50	**G. Hütter** A monolithic hyperintegrated ROM FE^2 method with clustered training strategy
09:50–10:15	**I. Plyushchay** Ab initio modeling of solid solution softening and hardening effects in Al-Mg-Zr-Si aluminum alloys and aluminum wrought alloys
10:15–10:40	**Coffee break**
10:40–11:05	**L. Dyckhof** Toward Hierarchical Modeling: Machine Learning for Describing Elastic-Plastic Behavior in Nanoporous Metals
11:05–11:30	**K. P. Abdolazizi** Viscoelastic Constitutive Artificial Neural Networks (vCANNs) – a framework for data-driven anisotropic nonlinear finite viscoelasticity
11:30–11:55	**R. Shoghi** Optimizing Machine Learning Yield Functions Using Active Learning for Support Vector Classification
11:55–12:20	**M. Harnisch** Enhancing data-driven inelasticity with neural networks: Opportunities in computational mechanics
12:20–13:30	**Lunch**
13:30–13:55	**K. A. Meyer** Thermodynamically consistent neural network plasticity modeling and discovery of evolution laws
13:55–14:20	**M. Abendroth** A Hybrid Approach to Model the 3D Inelastic Deformation Behavior of Cellular Media Using Neural Networks
14:20–14:45	**K. A. Kalina** Physics-augmented neural networks for constitutive modeling of elasticity and viscoelasticity
14:45–15:00	**Closing**
15:00	**Coffee and Farewell**

	Wednesday late afternoon, February 07, 2024 (optional!)
15:00–16:00	**Coffee**
16:00–16:20	**D. Melching**
	Incentive presentation: GAMM AG Phase-field meets GAMM AG Data
16:20–18:00	**All particitpants**
	Discussion
19:00–?	**Joint dinner**

3 Participants

Local organizers

- Dr. Karl Kalina, Institute of Solid Mechanics, TU Dresden, karl.kalina@tu-dresden.de
- Prof. Markus Kästner, Institute of Solid Mechanics, TU Dresden, markus.kaestner@tu-dresden.de
- Lennart Linden, Institute of Solid Mechanics, TU Dresden, lennart.linden@tu-dresden.de
- Alexandra Otto, Institute of Solid Mechanics, TU Dresden, alexandra.otto@tu-dresden.de
- Alexander Raßloff, Institute of Solid Mechanics, TU Dresden, alexander.rassloff@tu-dresden.de
- Paul Seibert, Institute of Solid Mechanics, TU Dresden, paul.seibert@tu-dresden.de

Participants

- Kian Abdolazizi, Institute for Continuum and Material Mechanics, Hamburg University of Technology, kian.abdolazizi@tuhh.de
- Dr. Martin Abendroth, Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, martin.abendroth@imfd.tu-freiberg.de
- Dr. Jörg Brummund, Institute of Solid Mechanics, TU Dresden, joerg.brummund@tu-dresden.de
- Lena Dyckhoff, Institut für Wasserstofftechnologie, Helmholtz-Zentrum Hereon, lena.dyckhoff@hereon.de
- Prof. Felix Fritzen, Institute of Applied Mechanics (CE) & SC SimTech, Data Analytics in Engineering (DAE), University of Stuttgart, fritzen@simtech.uni-stuttgart.de
- Prof. Sibylle Gemming, Institut für Physik, TU Chemnitz, sibylle.gemming@physik.tu-chemnitz.de
- Claudius Haag, Institute of Applied Mechanics, University of Stuttgart, claudius.haag@mib.uni-stuttgart.de
- Marius Harnisch, Institute of Mechanics, TU Dortmund, marius.harnisch@tu-dortmund.de
- Dr. Geralf Hütter, Institut für Bauingenieurwesen, Brandenburgische Technische Universität Cottbus - Senftenberg , geralf.huetter@b-tu.de
- Sanath Keshav, DAE, University of Stuttgart, keshav@mib.uni-stuttgart.de
- Dominik Klein, Cyber-Physical Simulation Group, Technical University of Darmstadt, klein@cps.tu-darmstadt.de
- Prof. Benjamin Klusemann, Leuphana University & Hereon, benjamin.klusemann@leuphana.de
- Mark Körbel, Cyber-Physical Simulation Group, Technical University of Darmstadt, mark.koerbel@web.de
- Nils Lange, Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, nils.lange@imfd.tu-freiberg.de
- David Melching, Institute of Materials Research, German Aerospace Center (DLR), david.melching@dlr.de
- Dr. Knut-Andreas Meyer, Institute of Applied Mechanics, TU Braunschweig, k.a.meyer@tu-braunschweig.de
- Abel Milor, Institute of Scientific Computing, TU Dresden, abel_henri_guillaume.milor@tu-dresden.de
- Prof. Inna Plyushchay, Faculty of Physics, Taras Shevchenko National University of Kyiv, inna.pl@knu.ua
- Max Rosenkranz, Chair of Scientific Computing for Systems Biology, TU Dresden, max.rosenkranz@tu-dresden.de

- Jan Schmidt, Interdisciplinary Center for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, jan.schmidt-p2d@rub.de
- Lena Scholz, DAE, University of Stuttgart, scholz@mib.uni-stuttgart.de
- Jasper Schommartz, Cyber-Physical Simulation Group, Technical University of Darmstadt, schommartz@cps.tu-darmstadt.de
- Ronak Shoghi, ICAMS, Ruhr-University Bochum, Ronak.Shoghi@ruhr-uni-bochum.de
- Matthias Thimm, Lehrstuhl für Festkörpermechanik, Department Maschinenbau, Universität Siegen, Matthias.Thimm@uni-siegen.de
- Basavesh Yaraguntappa, Institute of Applied Mechanics (CE), Chair I, University of Stuttgart, basavesh.yaraguntappa@mib.uni-stuttgart.de
- Zhengqing Wei, Institut für Physik, TU Chemnitz, zhengqing.wei@physik.tu-chemnitz.de

4 Abstracts

4.1 A physics-enhanced, neural network based modeling approach for hyperelastic beams

Jasper O. Schommartz*, Juan C. Alzate Cobo, Dominik K. Klein, Oliver Weeger

Institute Cyber-Physical Simulation, Technical University of Darmstadt, Germany;
mail: schommartz@cps.tu-darmstadt.de

Recent advances in additive manufacturing have led to increasing interest in designing truss-based lattice metamaterials, as they enable unique combinations of material properties, which can be optimized and tailored for a large variety of applications. However, efficient numerical modeling of the nonlinear material behavior, especially on beam level, remains an ongoing challenge. In particular, beam theories typically assume linear elasticity, while hyperelasticity can only be included by using geometrically exact beam models and through the numerically expensive computation of cross-sectional deformation [1] In this contribution a neural network (NN) based material model for hyperelastic beams is presented. It exploits the nonlinear, high-dimensional interpolation capabilities of NNs and captures the material response directly through stress and strain measures without requiring numerical integration over the cross-section. Thermodynamic consistency and the normalization criteria are fulfilled through the use of Sobolev training and normalization terms, respectively. Furthermore, extensions for beams with point symmetric cross-sections and a parameterization with the radius are presented.

The model was calibrated and trained on concentrically sampled data sets, where the stress measures are computed from solutions of the cross-sectional warping problem [1]. The warping problem was implemented in the Python package FEniCS and solved with the finite element method. The NN model yields excellent approximations for strain amplitudes up to 0.5 and good accuracy for even larger strains. The radius-parameterized model achieves good predictions for radius to length radios greater 0.04.

References

[1] A. Arora, A. Kumar, P. Steinmann [2019]: "A computational approach to obtain nonlinearly elastic relations of special Cosserat rods", Computer Methods in Applied Mechancis and Engineering **350**, 295–314

[2] L. Linden, D. K. Klein, K. A. Kalina, J. Brummund, O. Weeger, M. Kästner [2023]: "Neural networks meet hyperelasticity: A guide to enforcing physics", Journal of the Mechancis and Physics of Solids **179**, 105363

4.2 Automated constitutive modeling of hyperelastic solids based on physics-augmented neural networks

L. Linden[1,*], K. A. Kalina[1], J. Brummund[1], M. Kästner[1]

[1]: Institute of Solid Mechanics, Chair of Computational and Experimental Solid Mechanics, TU Dresden, Germany

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

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

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

References

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

[2] Linden, L., Klein, D. K., Kalina, K. A., Brummund, J., Weeger, O. and Kästner, M., Neural networks meet hyperelasticity: A guide to enforcing physics, Journal of the Mechanics and Physics of Solids 179 (2023)

[3] Kalina, K. A., Linden, L., Brummund, J. and Kästner, M., FE^{ANN}: an efficient data-driven multiscale approach based on physics-constrained neural networks and automated data mining, Journal of Computational Mechanics 71 (2023).

4.3 Stochastic hyperelastic constitutive modeling with Bayesian neural networks

M. Körbel, D. K. Klein, O. Weeger

Cyber-Physical Simulation, Technical University of Darmstadt, Germany.
mail: {klein,weeger}@cps.tu-darmstadt.de

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 (PANNs), circumventing the current limitations of analytically formulated material models.

In the present work, stochastic Bayesian neural networks (BNNs) are applied to model hyperelastic material behavior. Extending the PANN model introduced in [1] by stochasticity, the proposed model fulfills all common constitutive conditions of hyperelasticity by construction. Using BNNs instead of standard feed-forward neural networks (FFNNs) allows the model to represent uncertainty in the data it is calibrated to. Furthermore, it enables the assessment of uncertainties in the calibrated model, thus enhancing the interpretability of model predictions. Two different BNN architectures, which are both based on FFNNs, are investigated. The applicability of the models is demonstrated by calibrating them to data generated with an analytical potential.

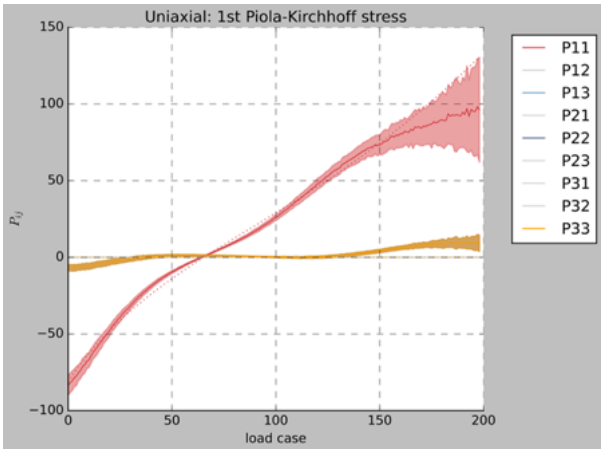


Figure 1: Stochastic PANN model prediction of uniaxial tension including extrapolation.

References

[1] L. Linden, D. K. Klein, K. A. Kalina, J. Brummund, O. Weeger, M. Kästner [2023]: "Neural networks meet hyperelasticity: A guide to enforcing physics", JMPS 179:105363.

4.4 Neural networks meet hyperelasticity: On limits of polyconvexity

D. K. Klein[1,*], L. Linden[2], K. A. Kalina[2], R. Ortigosa[3], M. Kästner[2], O. Weeger[1]

[1]: Cyber-Physical Simulation, Technical University of Darmstadt, Germany.
[2]: Institute of Solid Mechanics, Technical University of Dresden, Germany.
[3]: Multiphysics Simulation and Optimization, Technical University of Cartagena, Spain.
[*]: Corresponding author, *mail:* klein@cps.tu-darmstadt.de

In recent years, various constitutive modeling approaches based on neural networks (NNs) have emerged. It is widely agreed that the models should be formulated to fulfill physical and mathematical constitutive conditions such as objectivity and thermodynamic consistency. These *physics-augmented neural network* (PANN) approaches combine the extraordinary flexibility of NNs with a sound mechanical basis. This leads to reliable model predictions and allows for a model calibration with sparse training data. For hyperelastic material behavior, polyconvexity is one very promising constitutive condition to consider in PANN models. Polyconvexity implies ellipticity, which ensures stable simulations when applying the constitutive model in numerical applications. In [1], a polyconvex hyperelastic PANN model based on polyconvex invariants and convex neural network architectures was proposed. In [2], this model was extended by polyconvex normalisation terms, resulting in a hyperelastic PANN model which fulfills all constitutive conditions of hyperelasticity including polyconvexity by construction.

While polyconvex PANN models have been successfully applied to represent microstructured materials [1], in other cases, the assumption of polyconvexity was too restrictive [3]. Polyconvexity sets constraints such as convexity on the hyperelastic energy potential, which might not always incline with the actual observed material behavior. In such cases, using polyconvex models leads to insufficient model qualities. In the present work, polyconvex PANN models are calibrated to different microstructured materials to study and understand these limits of polyconvexity.

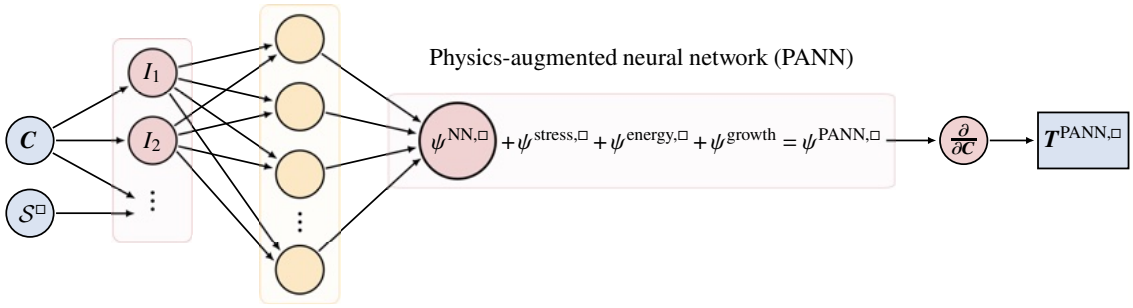


Figure 2: Hyperelastic physics-augmented neural network model [2].

References

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

[2] L. Linden, D. K. Klein, K. A. Kalina, J. Brummund, O. Weeger, M. Kästner [2023]: "Neural networks meet hyperelasticity: A guide to enforcing physics", JMPS 179:105363.

[3] D. K. Klein, R. Ortigosa, J. Martínez-Frutos, O. Weeger [2023] "Nonlinear electro-elastic finite element analysis with neural network constitutive models", Pre-print under review.

4.5 Inverse design of spinodoids from sparse data through Bayesian optimization

A. Raßloff[1], P. Seibert[1], K.A. Kalina[1], M. Kästner[1,2]

[1]: Institute of Solid Mechanics, TUD Dresden University of Technology, Germany; *mail:* alexander.rassloff@tu-dresden.de

[2]: Dresden Center for Computational Materials Science, TUD Dresden University of Technology, Germany

In this contribution, we propose a general framework to inversely designing structures using structure-property linkages. For deriving profound correlations, large databases are necessary. Experiments alone are prohibitively expensive. Therefore, computational augmentation is employed to allow for data-driven approaches even in this data scarce regime. In an iterative approach *(1)* mesostructures are characterized by descriptors, *(2)* effective properties are derived from numerical simulations, *(3)* structure-property linkages are set up using a Gaussian process, *(4)* descriptors of new candidates mesostructures are proposed by Bayesian optimization and *(5)* mesostructures are reconstructed. Steps 2 through 5 are repeated until a desired convergence criterion is reached, e.g., the uncertainty of the structure-property linkage is decreased or a mesostructured with preferable properties is found. This framework is applied and presented at the example of spinodoid structures. Augmenting a small initial data set by in silico reconstructed microstructures and their simulated effective properties allows for deriving improved structure-property linkages and, thus, finding potentially optimal microstructures or predicting properties.

4.6 Recent progress and challenges in descriptor-based microstructure reconstruction

P. Seibert[1], A. Raßloff[1], K. Kalina[1], M. Kästner[1,2]

[1]: Institute of Solid Mechanics, Dresden University of Technology, Germany
[2]: Dresden Center for Computational Materials Science, Dresden University of Technology, Germany
mail: markus.kaestner@tu-dresden.de

Microstructure reconstruction and characterization (MCR) provides realistic microstructure realizations for multiscale simulation and accelerating materials engineering. Common use-cases are

1. creating a 3D computational domain from 2D data such as a microscopy image,
2. reconstructing a small, periodic domain from a large, aperiodic CT scan,
3. creating a set of statistical volume elements from a single reference, and
4. enhancing microstructure datasets by sampling and interpolating in the descriptor space.

The first and penultimate case are demonstrated by means of concrete examples. Moreover, the last use-case enables data-driven materials design in data-scarce applications, as outlined in a separate contribution by A. Raßloff.

Descriptor-based MCR is a subclass of methods that aims at accomplishing all of these four goals. After a brief introduction to the underlying concepts, the potential of differentiable descriptors is analyzed in depth. Naturally, it makes the use of gradient-based optimization algorithms possible, reducing the number of iterations by orders of magnitude when compared to the Yeong-Torquato algorithm [1, 2]. This is discussed alongside with a validation, an implementation [3] and various extensions, e.g. for structures with fixed inclusion shapes, for an extremely scalable application of use-case (3) as well as a gradient projection based solution for use-case (1). As an outlook, current challenges are outlined in order to stimulate a discussion.

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

4.7 Influence of grain boundaries on the overall diffusivity in polycrystalline solids

L. Scholz[1], F. Fritzen[2]

[1]: Data Analytics in Engineering (Institute of Applied Mechanics), University of Stuttgart, Germany; *mail:* scholz@mib.uni-stuttgart.de
[2]: Data Analytics in Engineering (Institute of Applied Mechanics), University of Stuttgart, Germany; *mail:* fritzen@mib.uni-stuttgart.de

Major progress in battery technology is a key to the decarbnoization of industry and everyday life. All-Solid State Lithium Ion Batteries are based on a polycrystalline solid-state electrolyte. An in-depth understanding of the charateristics that govern Li ion diffusion within the solid electrolyte is crucial in order to understand how its performance can be improved.

In the literature the details of the polycrystalline structure on larger scales are often neglected or only considered under strong assumptions. However, the results of studies on smaller scale indicate that grain boundary effects do have a significant impact on the overall diffusivity but go along with massive computational demands. Hence, data-integrated approaches are essential for bringing the concepts on the different scales as well as computational and experimental results closer together.

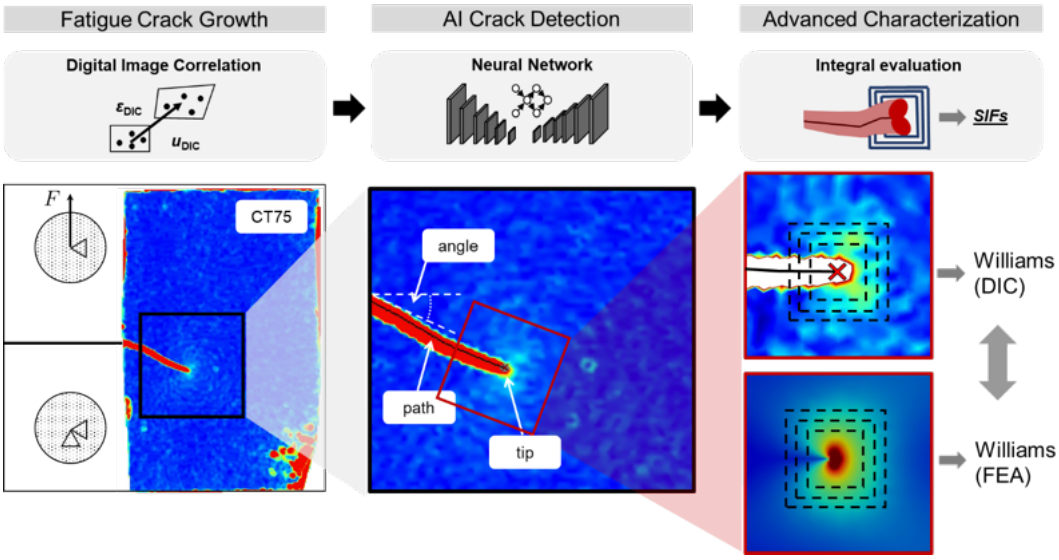
Our approach considers the fully resolved crystalline structure in a finite element setting where we use a novel interface element to account for diffusion along and across grain boundaries. By means of homogenization an effective model on the mesoscale is derived. The contribution of the grain boundary to the overall diffusivity can then be studied quantitatively. An in-depth analysis on the material and structural features governing the effective diffusion behavior in this model enables the design of meaningful surrogate models and helps us to find ways to reduce the computational cost across the space of input parameters. This will facilitate in silico exploration of microstructures and their implications on larger scales which, at a later stage, can be used to design improved batteries.

4.8 Advanced fracture mechanical analysis using digital image correlation, explainable machine learning, and data science

D. Melching[1], T. Strohmann[1], F. Paysan[1], E. Dietrich[1], G. Requena[1,2], E. Breitbarth[1]

[1]: Institute of Materials Research, German Aerospace Center (DLR), Germany; *mail:* david.melching@dlr.de
[2]: Metallic Structures and Materials Systems for Aerospace Engineering, RWTH Aachen University, Germany.

In recent years, digital image correlation (DIC) has become instrumental for contactless generation of full field surface displacements and strains during fatigue crack growth (FCG) experiments. Coupled with suitable material models, the DIC data can be used to determine important fracture parameters like stress intensity factors (SIFs). FCG mechanics is mainly driven by the crack tip field which can be described by the famous Williams series who's first order term relates to the $r^{-1/2}$ stress singularity and is used to determine K_I and K_{II}. Although the potential influence of higher order terms on crack growth and stability is known, classical studies solely rely on first order terms.



In this work, we present a framework for the characterization of crack tip fields taking higher-order terms into account and combine it with machine learning and a data-centric analysis. The framework is based on the following steps:

1. FCG experiments accompanied by robot-assisted DIC [1]
2. Automatic crack detection using trained convolutional neural networks and explainable AI [2]
3. Determination of Williams coefficients using the Python package *CrackPy* [3, 4]

We analyzed FCG experiments with compact tension (CT) specimens of aluminium AA7010 alloys and learned microstructure-dependent crack propagation laws from the data.

References

[1] F. Paysan, E. Dietrich, E. Breitbarth [2022]: "A Robot-Assisted Microscopy System for Digital Image Correlation in Fatigue Crack Growth Testing", Experimental Mechanics **63**, 975–986

[2] D. Melching, T. Strohmann, G. Requena, E. Breitbarth [2022]: "Explainable machine learning for precise fatigue crack tip detection", Scientific Reports **12**, 9513

[3] D. Melching, E. Breitbarth [2023]: "Advanced crack tip field characterization using conjugate work integrals", International Journal of Fatigue **169**, 107501

[4] T. Strohmann, D. Melching, F. Paysan, A. Klein, E. Dietrich, G. Requena, E. Breitbarth [2022]: "Crack Analysis Tool in Python - CrackPy (1.0.2)", https://doi.org/10.5281/zenodo.7472202

4.9 Knowledge-constrained splines for the prediction of physical phenomena

C. Haag[1], M.-A. Keip[2] and F. Fritzen[2]

[1]: University of Stuttgart, Institute of Applied Mechanics (CE), Pfaffenwaldring 7, 70569 Stuttgart; *mail:* claudius.haag@mib.uni-stuttgart.de

[2]: University of Stuttgart, Institute of Applied Mechanics (CE), Pfaffenwaldring 7, 70569 Stuttgart;

Magnetorheological elastomers (MREs) are composite materials comprised of elastomer matrix and magnetic inclusions [1]. In periodic structures, the magneto-mechanical response can be exploited to induce buckling-type structural instabilities that give rise to an abrupt change in their microscopic morphology [4].

The detection of the related instability points together with the resulting buckling patterns is an elaborate and time-consuming process. It is thus our goal to create a surrogate model that can predict the associated effects in an accelerated manner and with a reduced footprint concerning direct computational resources. We study the macroscopic bifurcation behavior of MRE microstructures [4] as a starting point.

We present a general spline-based computational approach for the prediction of physical phenomena that integrates quantitative (discrete, data-based) and qualitative (axiomatic, feature-based) evidence and information. For this approach, a new software-package for flexible spline-based regression is proposed: It enables to complement the available data by constraining the ansatz space by physical conditions. While the former are obtained from observation and given quantitatively (but potentially subjected to uncertainty and noise), the latter can be incorporated qualitatively through explicit function and parameter constraints, wiggle-constraints [2] or general non-linear constraints. Our spline software package aims at fulfilling the need for a general Python spline package within the FOSS community build on top of a comprehensive foundation incorparating extensive documentation, a test-suite and performance benchmarks.

As examples we consider three applications: First, a mechanical problem with partial unknowns is solved to solve an inverse problem. We reconstruct either the unknown cross-section area $A(x)$ or Young's modulus $E(x)$ from noisy samples of the displacement field. Second, we apply our software toolchain to discrete and unknown statistical data in order to identify the best probability density function (PDF) and its parameters. In this context we minimize the Kullback-Leibler divergence [3] of parameterized PDFs against our spline regressor. Third, analytical expressions of instability landscapes [4] will be generated by least-squares minimization [5] taking into account both, numerically obtained datasets of instability points and a-priori known physical features. The effect of the latter is the possibility to rely on much scarcer datasets inducing pronounced computational savings.

References

[1] Danas, K., Kankanala, S. V., Triantafyllidis, N. Experiments and modeling of iron-particle-filled magnetorheological elastomers. Journal of the Mechanics and Physics of Solids 60, pp. 120–138. 2012

[2] Duchon, J. Splines minimizing rotation-invariant semi-norms in Sobolev spaces. Lecture Notes in Mathematics 571, pp. 85–100, 1977.

[3] Kullback, S. and Leibler, R.A. On Information and Sufficiency. The Annals of Mathematical Statistics 22, pp. 79–86, 1951.

[4] Polukhov, E. and Keip, M.-A. Multiscale stability analysis of periodic magnetorheological elastomers. Mechanics of Materials 159, 103699, 2021.

[5] Wahba, G. Spline models for observational data. Society for Industrial and Applied Mathematics, 1990.

4.10 A Texture-Dependent Yield Criterion

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

[1]:ICAMS, Ruhr-University Bochum, Germany; *mail:* jan.schmidt-p2d@rub.de

Constitutive modeling of anisotropic plastic material behavior traditionally follows a deductive scheme, relying on empirical observations that are cast into analytic equations, the so-called phenomenological yield functions. Recently, data-driven constitutive modeling has emerged as an alternative to phenomenological models as it offers a more general way to describe the material behavior with no or fewer assumptions. In data-driven constitutive modeling, methods of statistical learning are applied to infer the yield function directly from a data set generated by experiments or numerical simulations. Currently these data sets solely consist of stresses and strains, considering the microstructure only implicitly. Similar to the phenomenological approach, this limits the generality of the inferred material model, as it is only valid for the specific material employed in the virtual or physical experiments.

In this work, we present an approach to overcome this limitation by incorporating explicitly microstructural information into the yield function. The approach builds upon the support vector machine (SVM) for ideal plasticity [2] and extends its feature space from stress only to stress + texture. The texture is described by the coefficients of the general spherical harmonics (GSH) series expansion of the orientation distribution function. We create a data set that contains the yield points in 300 different directions for over 7000 textures by using full-field crystal plasticity simulations. A single SVM classifier is trained on this data set to find the class boundary between elastic and plastic data points dependent on stress and texture.

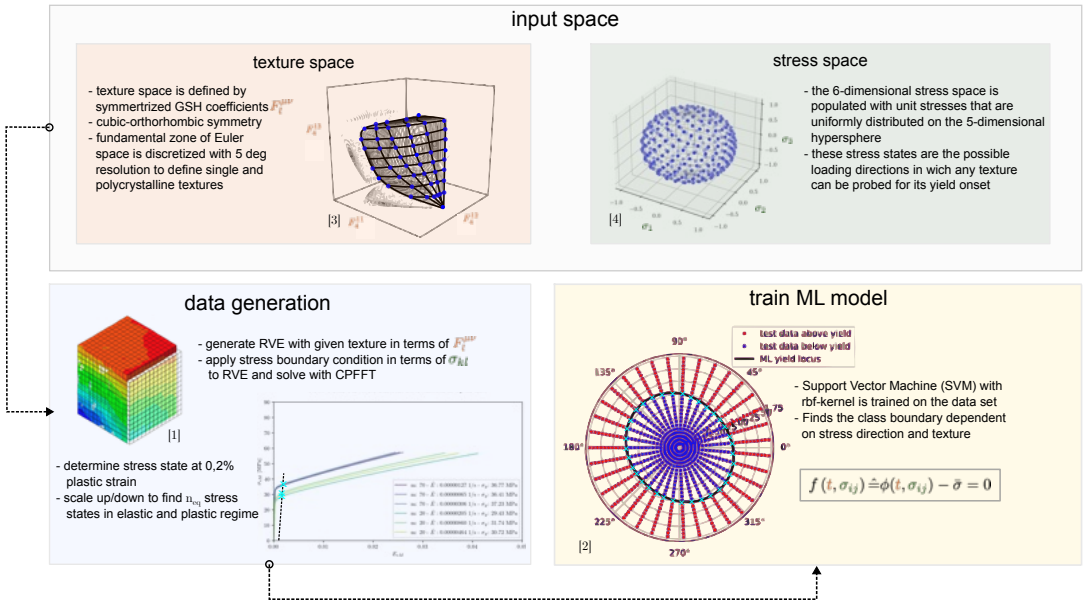


Figure 3: Finding a texture-dependent yield function. The input space is described by a stress direction (top right) and the GSH coefficients of the texture (top left). CP simulations are performed on an RVE to find the macroscopic yield point at 0.2 % plastic strain. The SVM classifier is trained on the emerging data set of stresses and GSH coefficients to find the class boundary between elastic and plastic data points.

References

[1] A. Biswas et al [2022]: "A hybrid approach for the efficient computation of polycrystalline yield loci with the accuracy of the crystal plasticity finite element method", Modelling Simul. Mater. Sci. Eng. **30**.

[2] A. Hartmaier [2020]: "Data-Oriented Constitutive Modeling of Plasticity in Metals", Materials 13,**7**: 1600.

[3] G. Proust, S.R. Kalidindi [2006]: "Procedures for construction of anisotropic elastic-plastic property closures for face-centered cubic polycrystals using first-order bounding relations", J. Mech. Phys. Solids, **54**: 1744-1762.

[4] R. Shoghi, A. Hartmaier [2022]: "Optimal Data-Generation Strategy for Machine Learning Yield Functions in Anisotropic Plasticity", Front. Mater., **9**: 868248.

4.11 Parameterized Nonuniform Transformation Field Anaylsis

Felix Fritzen[1], Julius Herb[1], Shadi Sharba[2]

[1]: Institute of Applied Mechanics (CE), Data Analytics in Engineering, University of Stuttgart, Germany; *mail:* fritzen@mib.uni-stuttgart.de, julius.herb@mib.uni-stuttgart.de

[2]: Fraunhofer ISC, Germany; *mail:* shadi.sharba@isc.fraunhofer.de

The Nonuniform Transformation Field Analysis [NTFA; 1, 2] has proven as powerful tool for the investigation of materials with history variables. By extending Dvorak's idea of piece-wise uniform transformation fields to spatially heterogeneous eigenstrains, the need for (many) subdomains has been eliminated. This leads to a modest number of reduced internal state variables while preserving accuracy, outstanding numerical efficiency and the possibility to reconstruct accurate local stress and strain information during postprocessing without the need for additional simulations.

One short-coming of the NTFA until today has been its restriction to constant elastic properties. These are needed in order to guarantee static compatibility of the so-called self-equilibrated modes that are at the heart of the NTFA. In reality the elastic properties can, however, depend on external influence factors, e.g., on the temperature θ, or on the history of the loading that the microstructure has undergone. We present a major extension of the NTFA by allowing for variable elastic properties. Therefore, we exploit our recent work on thermo-elastic homogenization [3] in which we use ideas from reduced order modeling and affine operator representation to produce an abundance of quality data. Further, we propose a look-up table for the NTFA based on this quality data. This staggered approach leads to a net online runtime that is on par with the classical NTFA despite the additional freedom in terms of full temperature dependence of the thermal eigenstrain and the elastic material properties. We demonstrate the efficiency of the approach on isolated RVE simulations as well as in full 3D twoscale simulations with hundreds of thousands of macroscopic degrees of freedom which still run on laptop computers. Our method is about to be submitted for publication [4].

References

[1] J.C. Michel, P. Suquet [2004]: *Computational analysis of nonlinear composite structures using the nonuniform transformation field analysis,* Computer Methods in Applied Mechanics and Engineering **193**, p. 5477-5502. doi: https://doi.org/10.1016/j.cma.2003.12.071

[2] F. Fritzen, T. Böhlke, E. Schnack [2010]: *Three-dimensional finite element implementation of the nonuniform transformation field analysis,* International Journal for Numerical Methods in Engineering International Journal for Numerical Methods in Engineering **84:7**, p. 803-829 , doi: https://doi.org/10.1002/nme.2920

[3] S. Sharba, J. Herb, F. Fritzen [2022]: *Reduced order homogenization of thermoelastic materials with strong temperature-dependence and comparison to a machine-learned model,* Archives Of Applied Mechanics **93**, p. 2855-2876. doi: https://doi.org/10.1007/s00419-023-02411-6

[4] F. Fritzen, J. Herb, S. Sharba [2024]: *Thermo-Plastic Nonuniform Transformation Field Analysis for Eigenstress Analysis of Laser Dispersed Materials*, in preparation

4.12 A monolithic hyperintegrated ROM FE^2 method with clustered training strategy

G. Hütter[1,2], N. Lange[1], B. Kiefer[1]

[1]: TU Bergakademie Freiberg, Germany; *mail:* Nils.Lange@tu-freiberg.de
[2]: Brandenburg University of Technology Cottbus-Senftenberg, Germany; *mail:* Geralf.Huetter@b-tu.de

Numerical homogenization methods are widely used in science and industrial applications to predict the effective behavior of engineering materials in structural components based on their microstructure. For nonlinear material behavior, this requires solving coupled boundary value problems for the microscale and macroscopic scale in a concurrent way. The most flexible approach for this purpose is the utilization of the finite element method on both scales, known as the FE^2 method [1]. The high flexibility and generality comes along with high computational costs, which motivated numerous techniques to reduce these costs. In particular, neural network (NN)-based surrogate models or reduced-order models (ROM) [2,3] have attracted a lot a research effort. Both types of models are driven by training data from expensive fully-resolved microscale simulations as their input. But while NN-based models need to be augmented to capture physical constraints, ROM-FE models form variational approximations to the microscale problem and thus inherit their fundamental physical behavior, though still at higher computational costs than surrogate models. The costs do not only comprise the online computational time during the actual structural simulation, but also the so-called offline costs for generating the training data.

The present contribution shows how a hyperintegrated ROM method can be combined with a monolithic solution strategy to reduce the online costs, in conjunction with a clustered training strategy to lower offline costs for generating training data. Certain 2D and 3D examples with highly nonlinear, irreversible material demonstrate the wide applicability of the method at minimal adaption effort to a specific problem.

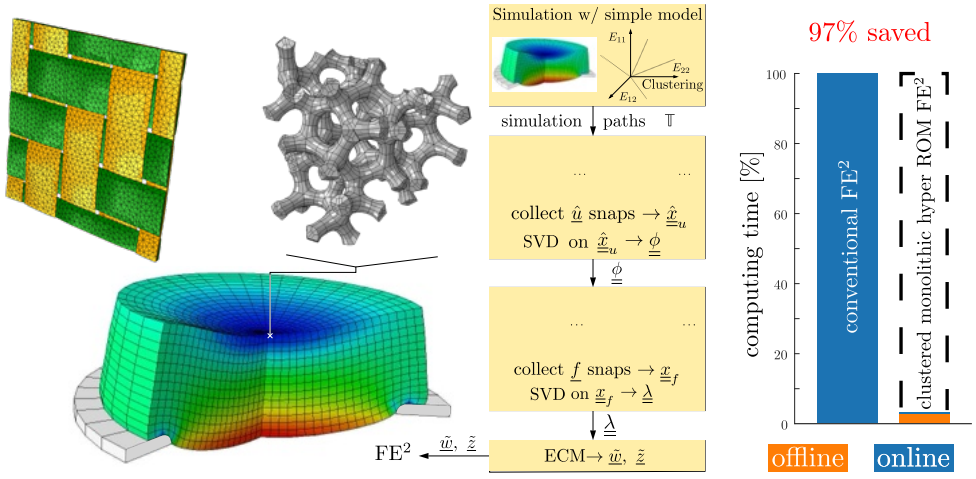


Figure 1: from [4]

References

[1] J. Schröder [2014]: "A numerical two-scale homogenization scheme: the FE^2-method", In: J. Schröder, K. Hackl (Eds.), Plasticity and Beyond: Microstructures, Crystal-Plasticity and Phase Transitions, Springer, Vienna, 1–64.

[2] F. Fritzen, M. Leuschner [2013]: "Reduced basis hybrid computational homogenization based on a mixed incremental formulation", Computer Methods in Applied Mechanics and Engineering **260**, 143–154.

[3] J.A. Hernández, J. Oliver, A.E. Huespe, M.A. Caicedo, J.C. Cante [2014]: "High-performance model reduction techniques in computational multiscale homogenization", Computer Methods in Applied Mechanics and Engineering **276**, 149–189.

[4] N. Lange, G. Hütter, B. Kiefer [2024]: "A monolithic hyper ROM FE^2 method with clustered training at finite deformations", Computer Methods in Applied Mechanics and Engineering **418**, 116522.

4.13 Ab initio modeling of solid solution softening and hardening effects in Al-Mg-Zr-Si aluminum alloys and aluminum wrought alloys.

I. Plyushchay[1,2], Z. Wei[1], S. Gemming[1]

[1]Institute of Physics, TU Chemnitz, Chemnitz, Germany; *mail:* sibylle.gemming@physik.tu-chemnitz.de
[2]Faculty of Physics, Taras Shevchenko National University of Kyiv, Ukraine *mail:* inna.pl@knu.ua

In classical modeling, solid solution hardening of alloys is attributed to mechanical stress fields around vacancies, substitutional atoms and dislocations, and to their influence on the elastic modulus of the alloy. In the present study, first-principles modelling of periodically repeated supercells allows us to go beyond this simple size argument and include also changes to the state of the electronic subsystem around point and line defects in aluminium alloys. The calculations were carried out using the DFT method in the GGA approximation using the ABINIT software package [1].

We systematically vary the relative arrangement of the defects within the supercell and the type of element included in the substitutional defect in order to provide data suitable for refining state-of-the-art machine learned potentials, which so far extend the traditional Hume-Rothery-based descriptors only by data from classical phase diagram calculations [2]. Our aim is to identify descriptors, which can be evaluated in a standard first-principles work flow in order to transfer the present approach to Al alloys with more complex compositions and, in the future, also to other base alloys.

In particular, the lattice distortion around substitutional Mg, Zr, and Si atoms and around the vacancy site in crystalline aluminum, as well as their interactions, were analyzed using supercells of various sizes. The results indicate that the radius of the first coordination sphere changes within a range of $\pm 1.5\%$. An in-depth analysis of lattice and electron density variations around an impurity atom indicates that all discernible changes in electron density are localized within the first coordination sphere surrounding the impurity. The calculation of the interaction between point defects indicates a potential tendency for the formation of MAl_3 (M = Mg, Zr) precipitates, which may promote precipitation strengthening in Al-Mg-Zr-Si aluminium alloys. When the impurity atom is placed in the vicinity of an edge dislocation core additional contributions to the commonly applied classical 'size-stress' theory are obtained, which show that the effect of electronic interactions needs to be included to refine the classical model. Second, the effect of the most common impurity atoms on the slip of edge dislocations in crystalline aluminium was studied as a fundamental mechanism of the plastic deformation, in particular of wrought Al alloys.

Acknowledgement: This work was funded by the Deutsche Forschungsgemeinschaft via RTG 2868 D^3, DATA-DRIVEN DESIGN OF RESILIENT METAMATERIALS, (Spokesperson Prof. Dr. Markus Kästner, TU Dresden, Project 493401063) and via a Scholarship by TU Chemnitz supporting the scientific visit of Prof. Dr. Inna Plyushchay.

References

[1] www.abinit.org

[2] S. Gao, Z. Gao. F. Zhao [2023]: "Machine learning and visualization assisted solid solution strengthening phase prediction of high entropy alloys", Materials Today Communications **35**, 105894.

4.14 Toward Hierarchical Modeling: Machine Learning for Describing Elastic-Plastic Behavior in Nanoporous Metals

L. Dyckhoff[1], N. Huber[1,2]

[1]: Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany; *mail:* lena.dyckhoff@hereon.de

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

Modeling hierarchical nanoporous metals, characterized by complex ligament networks across multiple length scales [1], is computationally demanding. Multiaxial stresses occur in higher hierarchy ligaments, which add to the complexity of the problem and require an understanding of multiaxial material behavior. For finite element (FE) modeling, we propose separating the hierarchical nanoporous structure into upper and lower levels, enabling an efficient analysis of structure-property relationships. To reduce computational cost, we aim to use surrogate models and FE-beam models for predicting the mechanical behavior of the lower level of hierarchy.

Our study focuses on idealized diamond FE-beam models representing the lower hierarchy, with yield surfaces exhibiting anisotropy. These surfaces are effectively described by data-driven techniques such as artificial neural networks and support vector classification (SVC) [2]. These methods are extended to predict yield surfaces after preloads [3]. Integrating the trained SVC into an Abaqus UMAT yielded promising results for small deformations under a non-associated flow rule. However, challenges arose regarding convergence in the plastic regime and predicting complex load histories. Thus, we redirected our focus to recurrent neural networks (RNN) for predicting the stress response directly from strain paths, incorporating load history. While this approach is not entirely new [4], its application to hierarchical modeling introduces novelty. Our findings show that these RNNs successfully predict the response for load paths within the higher-level ligaments, assuming incompressible material behavior. The extension of this approach to account for the compressible behavior of the lower level of hierarchy holds promising potential.

References

[1] S. Shi et al., Science 371, 1026-1033, 2021 **1**, 123–154

[2] L. Dyckhoff, N. Huber, International Journal of Mechanical Sciences 259, 108601

[3] N. Jaeschke, Master's thesis, TUHH, 2023

[4] C. Bonatti, D. Mohr, Journal of the Mechanics and Physics of Solids 158, 2022, 104697

4.15 Viscoelastic Constitutive Artificial Neural Networks (vCANNs) – a framework for data-driven anisotropic nonlinear finite viscoelasticity

Kian P. Abdolazizi[1,*], Kevin Linka[1], Christian J. Cyron[1,2]

[1]: Institute of Continuum and Material Mechanics, Hamburg University of Technology, Germany
[2]: Institute of Material Systems Modeling, Helmholtz-Zentrum Hereon, Geesthacht, Germany
*mail: kian.abdolazizi@tuhh.de

The constitutive behavior of polymeric materials is often modeled by finite linear viscoelastic (FLV) or quasi-linear viscoelastic (QLV) models [1]. These popular models are simplifications that typically cannot accurately capture the nonlinear viscoelastic behavior of materials. For example, the success of attempts to capture strain (rate)-dependent behavior has been limited so far. To overcome this problem, we introduce viscoelastic Constitutive Artificial Neural Networks (vCANNs), a novel physics-informed machine learning framework for anisotropic nonlinear viscoelasticity at finite strains [2]. vCANNs rely on the concept of generalized Maxwell models enhanced with nonlinear strain (rate)-dependent properties represented by neural networks. The flexibility of vCANNs enables them to automatically identify accurate and sparse constitutive models of a broad range of materials. To test vCANNs, we trained them on stress-strain data from Polyvinyl Butyral, the electro-active polymers VHB 4910 and 4905, and a biological tissue, the rectus abdominis muscle. Different loading conditions were considered, including relaxation tests, cyclic tension-compression tests, and blast loads. We demonstrate that vCANNs can learn to capture the behavior of all these materials accurately and computationally efficiently without human guidance.

References

[1] K. Linka et al. [2021], "Unraveling the local relation between tissue composition and human brain mechanics through machine learning", Frontiers in Bioengineering and Biotechnology **9**, https://doi.org/10.3389/fbioe.2021.704738.

[2] K.P. Abdolazizi, K. Linka, C.J. Cyron [2023], "Viscoelastic Constitutive Artificial Neural Networks (vCANNs) - a framework for data-driven anisotropic nonlinear finite viscoelasticity", Journal of Computational Physics, in press, https://doi.org/10.1016/j.jcp.2023.112704.

4.16 Optimizing Machine Learning Yield Functions Using Active Learning for Support Vector Classification

R. Shoghi [1], L. Morand [2], D. Helm [2], A. Hartmaier [1]

[1]: Interdisciplinary Center for Advanced Materials Simulation (ICAMS), Bochum, Germany;
[2]: Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany;

Machine Learning (ML) methods are increasingly being recognized as powerful tools in the development of data-driven constitutive models. These models can describe complex material behavior in a more flexible way than classical constitutive models. The yield function, which is central to plasticty models, can be effectively formulated using ML techniques. The effectiveness of these models relies on the availability of comprehensive, high-quality training data, which is typically sourced from numerical simulations, experiments, or a combination of both. In this work, an active learning strategy using Support Vector Classification (SVC) has been introduced for the training of an ML-based yield function. This strategy employs the Query-By-Committee (QBC) algorithm to optimize the sampling of the stress space. The QBC algorithm facilitates the selection of new training data points in feature space, especially in regions where the committee of models shows considerable variations in their predictions. By identifying these areas of significant predictive divergence, the algorithm effectively selects key data points, ensuring a more comprehensive representation of the stress space. Notable reductions in the variance of model predictions and enhancements in the overall quality of the trained model have been achieved through this approach. For future work, we aim to integrate crystal-plasticity finite element method (CPFEM) simulations into the active learning framework. Such advancements are considered crucial in the development of digital material twins, providing a more comprehensive understanding of material behavior.

4.17 Enhancing data-driven inelasticity with neural networks: Opportunities in computational mechanics

M. Harnisch[1], T. Bartel[1], B. Schweizer[2], A. Menzel[1,3]
[1]: Institute of Mechanics, TU Dortmund University, Germany; *email:* marius.harnisch@tu-dortmund.de [2]: Chair I (Analysis), TU Dortmund University, Germany ; [3]: Division of Solid Mechanics, Lund University, Sweden

In recent years, various data-driven methods have been developed in the field of computational mechanics. Data-driven mechanics, introduced by Kirchdoerfer and Ortiz [1], replaces conventional material modeling with data-sets containing snapshots of stress and strain assumed to be sufficiently accurate representations of the underlying material behavior. Build on these snapshots, termed material states, and on states fulfilling equilibrium and kinematic compatibility, denoted mechanical states, is a distance function, the minimization of which with respect to both the material and mechanical states yields the boundary value problems' solution.

Originally introduced for elasticity, the extension to inelasticity poses a significant challenge. In this contribution, we introduce our extension [2,3], which we base on quantities denoted history surrogate and propagator allowing us to preserve the spirit of the original approach so that no real-time adjustments of the data-set are required. We achieve this by storing essential information of the history in the history surrogate and update this quantity at the end of each time step using the propagator. Finding suitable choices of these quantities can be challenging. By utilizing a Neural Network as propagator [3], we can let the Neural Network tackle this task autonomously without resorting to a material model.

We present simulations for both a neural network and an intuitive propagator. The focus is placed on a discussion of the obtained results and a comparison between the intuitive and neural network propagator is provided, cf. Fig. 1.

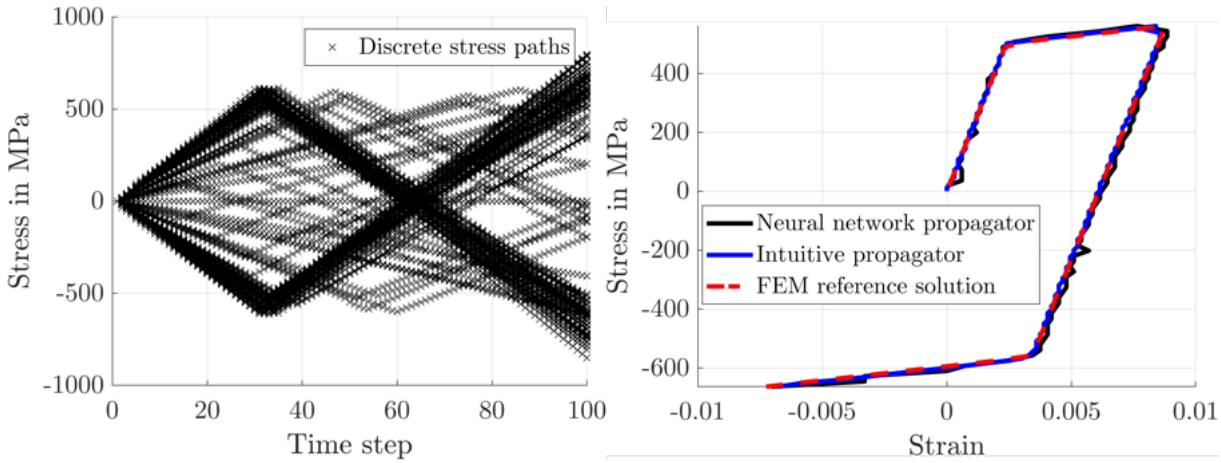


Figure 1: Left: Discrete stress paths which are used to construct the data-set. Right: Data-driven simulation using the constructed data-set. Results are shown using both an intuitive propagator (blue) and a neural network propagator (black), compared to a finite element reference solution (red).

References

[1] T. Kirchdoerfer, M. Ortiz, Data-driven computational mechanics, Comput. Methods Appl. Mech. Engrg. 304 (2016) 81-101

[2] T. Bartel, M. Harnisch, B. Schweizer, A. Menzel, A data-driven approach for plasticity using history surrogates: Theory and application in the context of truss structures, Comput. Methods Appl. Mech. Engrg. 414 (2023), 116-138

[3] K. Poelstra, T. Bartel, B. Schweizer, A data-driven framework for evolutionary problems in solid mechanics, J. Appl. Math. Mech (3) (2022)

4.18 Thermodynamically consistent neural network plasticity modeling and discovery of evolution laws

K. A. Meyer[1], F. Ekre[1], R. Jänicke[1]

[1]: Institute of Applied Mechanics, TU Braunschweig, Germany; *mail:* k.a.meyer@tu-bs.de

Over the past decade, advancements in computational frameworks and processing power have made deep neural networks increasingly viable for material modeling. However, purely data-driven models can yield non-physical predictions due to the lack of physical constraints. Physics-Informed Neural Networks (PINNs) incorporate physics into the training process, which partially address this issue but offer no guarantees outside the training data. As an alternative, a few recent works strictly enforce physics, which has been shown to generalize better [1].

In this contribution, we present a novel approach of strict enforcement that embeds the neural network within the material model, inherently fulfilling thermodynamic laws [2]. The network represents only the unknown physics allowing us to integrate knowledge accumulated from decades of constitutive modeling research into the data-driven methodology. By analyzing the trained, embedded networks, we recover existing evolution laws from artificial training data and discover new evolution laws from experimental data [3]. The discovered evolution laws for isotropic and kinematic hardening can qualitatively predict an experimentally observed yield strength evolution, which conventional evolution laws cannot describe.

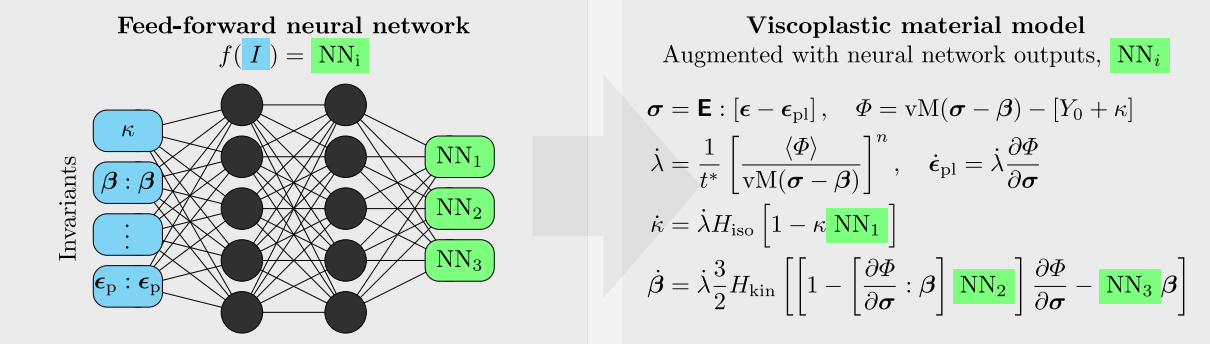


Figure 1: Neural Network embedded in viscoplastic evolution laws

References

[1] M. Rosenkranz, K. A. Kalina, J. Brummund, and M. Kästner [2023]: "A comparative study on different neural network architectures to model inelasticity", International Journal for Numerical Methods in Engineering, 1–39

[2] K. A. Meyer and F. Ekre [2023]: "Thermodynamically consistent neural network plasticity modeling and discovery of evolution laws", Journal of the Mechanics and Physics of Solids, **180**, 105416

[3] K. A. Meyer and J. Ahlström [2023]: "The role of accumulated plasticity on yield surface evolution in pearlitic steel", Mechanics of Materials, **179**, 104582

4.19 A Hybrid Approach to Model the 3D Inelastic Deformation Behavior of Cellular Media Using Neural Networks

M. Abendroth[1], A. Malik[2], G. Hütter[3], B. Kiefer[4]

[1]: TU Bergakademie Freiberg, Germany; *mail:* martin.abendroth@imfd.tu-freiberg.de
[2]: TU Bergakademie Freiberg, Germany; *mail:* alexander.malik@imfd.tu-freiberg.de
[3]: Brandenburg University of Technology Cottbus-Senftenberg, Germany; *mail:* geralf.huetter@b-tu.de
[4]: TU Bergakademie Freiberg, Germany; *mail:* bjoern.kiefer@imfd.tu-freiberg.de

Describing the inelastic deformation behavior of cellular media in a constitutive manner is challenging due to the strong dependency on the microstructure and its bulk material. The possible combination of isotropic, kinematic, and distortional hardening, as well as anisotropic, non-associated yielding, form a complex context. The yield surface, flow rule, and internal variable evolutions differ for various cellular foam structures. Due to this, a constitutive material model adapting changes in the microstructure and bulk material is required in a homogenized setting. To reduce computational effort and complexity, representative volume elements (RVE) of generic foam structures are investigated. Neural networks are trained from numerous finite element simulations of the loaded RVE to approximate the yield and flow potentials. The networks are incorporated in a hybrid approach to establish the material model to be compliant with thermodynamic principles. This contribution focuses on the requirements of the training data set, sampling strategy, and neural network properties, as well as implementation aspects for a robust model. To conclude the investigations, numerical effort and approximation accuracy are analyzed. As an example, the hybrid approach is applied to a three-dimensional open-cell foam structure with elastoplastic bulk material exhibiting isotropic hardening. Possible extensions of the presented approach are discussed in conclusion.

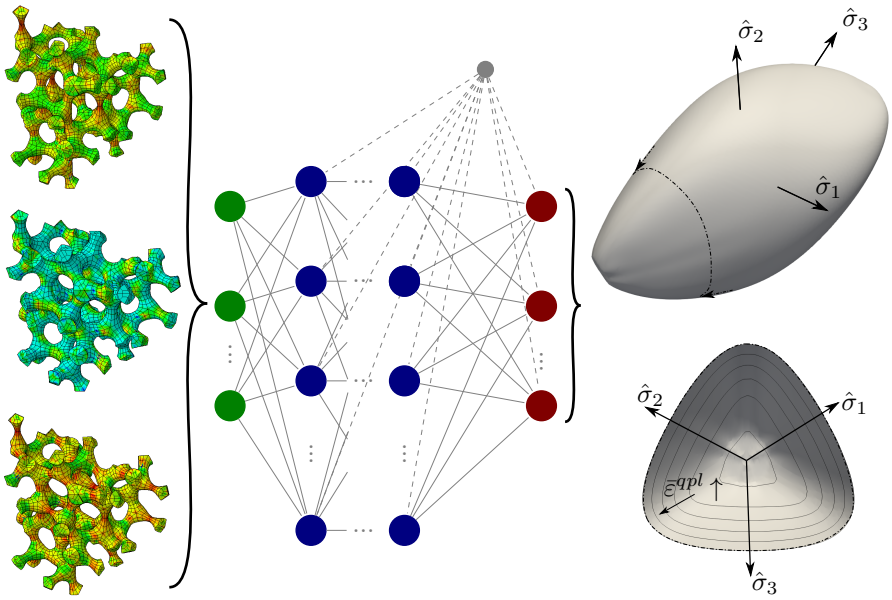


Figure 1: Yield surfaces and plastic flow directions are predicted by neural networks, which are trained with results of finite element simulations of representative volume elements representing cellular foam-like media.

References

[1] A. Malik, M. Abendroth, G. Hütter, B. Kiefer [2021]: "A hybrid approach employing neural networks to simulate the elasto-plastic deformation behavior of 3D-foam structures", Advanced Engineering Materials **1**, 2100641

[2] M. Abendroth, G. Hütter, C. Settgast, A. Malik, B. Kiefer, M. Kuna [2020]: "A hybrid approach to describe the elastic-plastic deformation behavior of porous media including damage effects", Technische Mechanik, **40**, 5-14

[3] C. Settgast, G. Hütter, M. Kuna, M. Abendroth [2019]: "A hybrid approach to simulate the homogenized irreversible elastic-plastic deformations and damage of foams by neural networks", International Journal of Plasticity, **126**, 102624

4.20 Physics-augmented neural networks for constitutive modeling of elasticity and viscoelasticity

K. A. Kalina[1], M. Rosenkranz[2], J. Brummund[1], W. Sun[3], M. Kästner[1]

[1]: Institute of Soild Mechanics, TU Dresden, 01062 Dresden, Germany; *mail:* karl.kalina@tu-dresden.de
[2]: Institute of Artificial Intelligence, TU Dresden, 01062 Dresden, Germany
[3]: Department of Civil Engineering and Engineering Mechanics, Columbia University, NY 10027, New York, United States

The formulation and calibration of constitutive models is still a challenging task for materials which exhibit complex nonlinear elastic or inelastic behavior. For this reason, data-driven methods and in particular the use of neural networks (NNs) have recently become increasingly popular. Thereby, NN-based approaches with integrated physical knowledge have shown to be particularly suitable.

In the first part of this contribution, we present an approach based on physics-augmented neural networks (PANNs) [1,2,3] that are applied as macroscopic surrogate models for expensive simulations of representative volume elements (RVEs). Our approach allows the efficient simulation of materials with complex underlying microstructures which reveal an overall anisotropic and nonlinear elastic behavior on the macroscale. By using a set of problem-specific invariants as the input of the PANN and the Helmholtz free energy density as the output, several physical principles, e.g., objectivity, material symmetry or thermodynamic consistency are fulfilled a priori [1]. The invariants are formed from structure tensors and the right Cauchy Green deformation tensor. Necessary data for the training of the PANN surrogate model are collected via computational homogenization of RVEs. Besides the network parameters, the structure tensors are automatically calibrated during training so that the underlying anisotropy of the RVE is reproduced in the best possible way. The developed approach is applied to several examples.

In the second part of this talk, a PANN approach for the modeling of viscoelastic materials is shown [4]. The model is built on the concept of generalized standard materials and is therefore thermodynamically consistent by construction. It consists of a free energy and a dissipation potential, which can be either expressed by the coordinates of their tensor arguments or by a suitable set of invariants. The two potentials are described by fully/partially input convex neural networks. For training of the model by paths of stress and strain, an efficient and flexible training method based on a recurrent cell is developed to automatically provide the internal variable(s) during the training process. The ability of the approach is shown in several descriptive examples.

References

[1] L. Linden, D. K. Klein, K. A. Kalina, J. Brummund, O. Weeger, M. Kästner [2023]: "Neural networks meet hyperelasticity: A guide to enforcing physics", Journal of the Mechanics and Physics of Solids **179**

[2] K. A. Kalina, L. Linden, J. Brummund, M. Kästner [2023]: "FE$^{\text{ANN}}$: an efficient data-driven multiscale approach based on physics-constrained neural networks and automated data mining"', Computational Mechanics **71**

[3] K. A. Kalina, P. Gebhart, J. Brummund, L. Linden, W. Sun, M. Kästner [2024]: "Neural network-based multiscale modeling of finite strain magneto-elasticity with relaxed convexity criteria", Computer Methods in Applied Mechanics and Engineering, **421**

[4] M. Rosenkranz, K. A. Kalina, J. Brummund, W. Sun, M. Kästner [2024]: "Viscoelasticty with physics-augmented neural networks: Model formulation and training methods without prescribed internal variables", Preprint, https://doi.org/10.48550/arXiv.2401.14270