Spotlights in Computational Physics and Engineering (SCoPE)

Invited lectures on:

Realistic RVEs by microstructure reconstruction: Basics, recent progress and challenges

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Abstract

One of the most important pillars supporting the digitization and acceleration of materials engineering at the continuum length scale is the ability to efficiently make use of the numerical tools that were developed in the last decades. While much research is focused on further refining constitutive models and numerical algorithms, an often-overlooked aspect is microstructure reconstruction and characterization (MCR). Specifically, MCR is needed for the following tasks:

1. creating a plausible 3D representative volume element (RVE) 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 and then reconstructing the corresponding microstructures.

While off-the-shelf machine learning methods can solve some of these tasks given a sufficiently large data set, descriptor-based reconstruction algorithms succeed at all four of them. Therein, the statistical microstructure morphology is quantified by so-called microstructure descriptors. Descriptor-based MCR has an advantage over machine learning-based MCR in that it does not need a data set. Instead, it can be used to create it, making data-driven modeling and simulation possible on otherwise insufficient amounts of data.

Four presentations à 30 minutes give an extensive introduction to the foundations of microstructure reconstruction and delve into recent progress and challenges achieved and faced by the authors. In particular, the following content is presented:

1. Introduction to microstructure descriptors and the Yeong-Torquato algorithm as well as gradient-based reconstruction from differentiable descriptors in 2D and 3D.
2. Case study on effective fracture properties and the relevance of MCR for statistical evaluation as well as a highly scalable approach where pattern generating PDE systems are learned from statistical descriptors by neural cellular automata.
3. Restriction to known geometries for specific material classes – brief literature review and gradient-based reconstruction of microstructures with ellipsoidal inclusions by analytical descriptors.
4. Open challenges including 3D scalability and polycrystalline structures and two recent ideas for approaching them – sequential gradient projection based on the Portilla-Simoncelli algorithm and continuously differentiable symmetrization of statistical descriptors for orientation map reconstruction

When and Where?

- 11.01.2024, 10:00-12:00, Maison du Nombre, MNO 1.030
- 12.01.2024, 10:00-12:00, Maison du Nombre, MNO 1.030

Invitee: Paul Seibert*

PAUL SEIBERT is a PhD Candidate at the Institute of Solid Mechanics at the **Technische Universtität Dresden** working on Microstructure characterization and reconstruction, and Structure-property-linkages.

Selected Publications

- P Seibert, A Raßloff, Y. Zhang, K Kalina, P. Reck, D. Peterseim, M Kästner; Reconstructing microstructures from statistical descriptors using neural cellular automata; IMMJ (accepted); 2023 P Seibert, M. Husert, M. Wollner, K Kalina, M Kästner; Fast reconstruction of microstructures with ellipsoidal inclusions using analytical descriptors; CADJ; 2023
- P Seibert, A. Raßloff, K Kalina, A. Safi, P: Reck, D: Peterseim, B. Klusemann , M Kästner; On the relevance of descriptor fidelity in microstructure reconstruction; PAMM; 2023
- P. Reck, P Seibert, A. Raßloff, M Kästner, D. Peterseim; Scattering transform in microstructure reconstruction; PAMM; 2023
- P Seibert, A Raßloff, K Kalina, J Gussone, K Bugelnig, M Diehl, M Kästner; Two-stage 2D-to-3D reconstruction of realistic microstructures: Implementation and numerical validation by effective properties; CMAME; 2023
- Y Zhang, P Seibert, A Otto, A Raßloff, M Ambati, M Kästner; DA-VEGAN: Differentiably Augmenting VAE-GAN for microstructure reconstruction from extremely small data sets; COMMAT; 2023
- C Düreth, P Seibert, D Rücker, S Handford, M Kästner; Conditional diffusion-based microstructure reconstruction; Materials Today Communications; 2023
- P Seibert, A Raßloff, K Kalina, M Ambati, M Kästner; Microstructure Characterization and Reconstruction in Python: MCRpy; Integrating Materials and Manufacturing Innovation; 2022
- P Seibert, A Raßloff, M Ambati, M Kästner; Descriptor-based reconstruction of three-dimensional microstructures through gradient-based optimization; Acta Materialia; 2022
- P Seibert, M Ambati, A Raßloff, M Kästner; Reconstructing random heterogeneous media through differentiable optimization; Computational Materials Science; 2021
- P Seibert, D Taylor, F Berto, SMJ Razavi; Energy TCD-robust and simple failure prediction unifying the TCD and ASED criterion; Engineering Fracture Mechanics; 2022
- P Seibert, L Susmel, F Berto, M Kästner, SMJ Razavi; Applicability of strain energy density criterion for fracture prediction of notched PLA specimens produced via fused deposition modeling; 2021
- P Seibert, SMJ Razavi, L Susmel, F Berto, M Kästner; Validation of the averaged strain energy density criterion for additively manufactured notched polylactide acid specimens; Procedia Structural Integrity; 2020