

ICAMS Special Seminar (online)

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Descriptor-based microstructure characterization and reconstruction: DMCR and MCRpy

Microstructure Characterization and Reconstruction (MCR) allows for (i) generating a plausible 3D computational domain from 2D information like a microscopy image, (ii) generating a set of statistical volume elements from a single representative example and (iii) augmenting microstructure datasets by sampling and interpolating in the descriptor space and subsequently reconstructing the corresponding structures. Two classes of reconstruction algorithms, descriptor-based and machine learning-based approaches, are distinguished and their advantages and disadvantages for computational materials engineering are compared.

After a formulation of the descriptor-based optimization problem, Differentiable MCR (DMCR) is presented. This recent approach achieves high efficiency without sacrificing expressivity by requiring the descriptors to be differentiable with respect to the microstructure parametrization. It can be accessed by MCRpy, a recently developed modular and extensible open-source software that facilitates microstructure characterization and descriptor-based reconstruction. MCRpy enables flexible combinations of descriptors, loss functions and optimizers and therefore implements a spectrum of reconstruction approaches ranging from the classical Yeung-Torquato algorithm to DMCR. Finally, current unpublished investigations are mentioned and future challenges are highlighted in order to stimulate a discussion about future projects and collaborations.

[1] Seibert, Ambati, Raßloff, Kästner, Reconstructing random heterogeneous media through differentiable optimization, *COMMAT*, 2021

[2] Seibert, Raßloff, Ambati, Kästner, Descriptor-based reconstruction of three-dimensional microstructures through gradient-based optimization, *Acta Materialia*, 2022

[3] Seibert, Raßloff, Kalina, Ambati, Kästner, Microstructure Characterization and Reconstruction in Python: MCRpy, *IMMJ*, 2022.