STATISTICAL 3D RECONSTRUCTION OF MICROSTRUCTURES FROM 2D DATA BY COMBINING STOCHASTIC GEOMETRY AND GENERATIVE AI

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This talk introduces a computational method for generating digital twins of the 3D morphology of (functional) materials through stochastic geometry models, calibrated by means of 2D image data. By means of systematic variations of model parameters a wide spectrum of structural scenarios can be investigated, such that the corresponding digital twins can be exploited as geometry input for numerical simulations of macroscopic effective properties [1,2,3]. For calibrating models that can generate virtual 3D microstructures by stochastic simulation, generative adversarial networks (GANs) have gained an increased popularity [4]. While GANs offer a data-driven approach for modeling complex 3D morphologies, the systematic variation of model parameters for generating diverse structural scenarios can be difficult. In contrast to this, relatively simple models of stochastic geometry (e.g., based on Gaussian random fields) allow parameter-driven structure variations, but can fall short in mimicking complex morphologies. Still, these "simple models" can be used to construct more advanced parametric stochastic geometry models (like excursion sets of more general random fields, or random tessellations induced by marked point processes). However, with increasing model complexity the calibration of model parameters to image data can become increasingly difficult. Combining GANs with advanced stochastic geometry models can overcome these limitations and, in addition, allows for the calibration of model parameters solely based on 2D image data of planar sections through the 3D structure [5]. These parametric hybrid models are flexible enough to stochastically model complex 3D morphologies, enabling the systematic exploration of different structures. Moreover, by combining stochastic and numerical simulations, the impact of morphological descriptors on macroscopic effective properties can be investigated and quantitative structure-property relationships can be established. Thus, the presented method, allows for the generation of a wide spectrum of virtual 3D morphologies, that can be used for identifying structures with optimized functional properties.

References

[1] B. Prifling et al. (2021). Front. in Mater. 8 (2021), 786502.
[2] O. Furat et al. (2021). npj Comput. Mater. 7, 105.
[3] E. Schlautmann et al. (2023). Adv. Energy Mater. 13, 2302309.
[4] S. Kench and S.J. Cooper (2021). Nat. Mach. Intell. 3, 299-305.
[5] L. Fuchs et al. (2024). Preprint. https://doi.org/10.48550/arXiv.2407.05333