Data-Driven Stereology: From 2D Images to Stochastic 3D Models of Material Microstructures

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Abstract

The functional performance of materials—such as those used in energy storage, filtration and biomedical applications—depends on their micro- and nanostructures. Establishing quantitative relationships between material processing parameters, structure and macroscopic properties remains a central challenge across materials science and related fields such as computational modeling, process engineering and materials informatics. Addressing this challenge typically requires three-dimensional information on the microstructure. However, the acquisition of 3D image data is often expensive, destructive and/or limited in resolution, motivating the development of computational approaches that infer 3D morphologies from more accessible 2D image data [1].

Recent advances in data-driven stereology have demonstrated that realistic 3D microstructures can be stochastically reconstructed from planar sections or 2D projections using generative methods from artificial intelligence (AI), particularly generative adversarial networks (GANs) [2,3]. Under certain mild assumptions such as isotropy, these computational models can learn the distribution of complex 3D morphologies directly from 2D image data and offer broad adaptability to different types of material microstructures and imaging modalities. However, these approaches are often not readily interpretable. More precisely, often AI-based methods involve a large number of learnable model parameters (weights), which makes them highly flexible but difficult to analyze or constrain physically. Their generality typically comes at the cost of requiring large and diverse training datasets to generate physically realistic and structurally accurate 3D morphologies. Without sufficiently comprehensive datasets, the generated morphologies may fail to exhibit physical plausibility, even if they appear statistically consistent with 2D training images.

In response to the challenges of interpretability and data efficiency in AI-based stereological methods, data-driven approaches can be combined with interpretable, parametric stochastic geometry models, such as random tessellations [4]. These models offer a mathematically grounded and interpretable framework for generating synthetic microstructures that adhere to physically meaningful morphological constraints.

This talk will present a computational framework that combines interpretable stochastic 3D models of stochastic geometry with generative AI techniques in order to facilitate model calibration by means of 2D image data. The methodology combines GAN-based training with models such as random tessellations (for modeling polycrystalline microstructures) [5], random fields on the unit sphere (for modeling particle surfaces) [6], and excursion sets of random fields (for modeling porous or multiphase materials) [7]. This combined approach enables the statistical reconstruction of physically plausible 3D microstructures from 2D imaging data. In this manner, measurement efforts can be significantly reduced in various scientific fields such as materials science, where high-resolution 3D imaging is often costly or experimentally constrained.

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