Parameter Estimation for Graph-based Stochastic Structure Models by Means of Convolutional Neural Networks

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Abstract

The combination of stochastic 3D modeling with numerical simulations of physical properties is a powerful tool for quantifying the impact of micro- or nanoscale morphology on macroscopic physical properties. For cathodes in solid oxide fuel cells (SOFCs), which consist of nickel, a ceramic phase, and pores, a graph-based stochastic 3D structure model was developed in [1] to reproduce the connectivity of all three phases. In the first step of the model, a random graph is generated independently for each phase in three-dimensional Euclidean space. In the second step, each point in space is assigned to the phase whose corresponding graph is closest to that point. Since the random graphs are parametric, the resulting structure model is also parametric. So far, model parameters have been estimated using minimum contrast estimation based on morphological descriptors. In this work, we present an alternative approach using convolutional neural networks with a U-net architecture [2]. Using simulated data, these networks are trained to extract the underlying graphs from model realizations, allowing for direct estimation of the model parameters. We evaluate the quality of these estimators and discuss the application of the trained networks to slightly generalized stochastic 3D structure models.

References

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