GRAPH CONVOLUTIONAL NEURAL NETWORKS FOR MODELING MATERIALS WITH MICROSTRUCTURE

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ABSTRACT

Predicting the evolution of a representative sample of a material with microstructure is a fundamental problem in homogenization. In this work we propose a graph convolutional neural network that utilizes the discretized representation of the initial material microstructure directly, without segmentation or clustering which might be occluded by noise in real data. This framework preserves rotational invariance like other graph-based convolutional neural networks, it works natively on both unstructured and structured grid data, and it does not require featurization of the multi-channel/hyperspectral image data. While it can benefit from obvious features, no feature engineering is needed to obtain good accuracy. We demonstrate the performance of the proposed network and compare it to traditional pixel-based convolution neural network models and feature-based graph convolutional neural networks on {multiple} large datasets.