Innovative Machine Learning Approaches for Predicting the Dynamics of the Phase-Field Microstructures

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The phase-field model is a well-known mesoscopic computational framework for predicting various phase change processes such as spinodal decomposition, thin-film deposition, and crack propagation. Advanced numerical methods that tackle the nonlinearity and higher-order derivatives in the governing equations are computationally expensive. Therefore, researchers have attempted to leverage the power of machine learning techniques to solve the phase-field model. Nevertheless, the spinodal decomposition data chosen to train the neural network are typically in the late domain growth stage without considering the early-stage decomposition dynamics. In this work, we compare two approaches to analyzing a binary-component spinodal decomposition dataset that includes late and early-stage behaviors. The data are generated using the Cahn-Hilliard equation with the Flory-Huggins free energy function and concentration-dependent mobility. The parallelized semi-implicit Fourier spectral method accelerates the solver to produce high-resolution input data. Two protocols are separately applied with 4500 training and 500 validation datasets of morphological evolutions. First, we implement PredRNN[1] to capture the underlying temporal and spatial correlations. With cheap 2D convolution on the spatial dimension and a new memory decoupling loss, PredRNN can more readily capture both short and long-term memory simultaneously. In the second approach, we apply the dimensional reduction process with statistic representation on the phase field dataset.[2] Moreover, attention mechanism is applied to improve output performance. We expect the new machine learning models to predict much more accurate low-dimensional results than the traditional model, enhancing the correctness of later reconstruction.

Reference

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