Spatiotemporal Machine-Learning Prediction for the Evolution of Phase-Field Microstructures

Sheng-Jer Chen[a] and Hsiu-Yu Yu[a*]

[a] Department of Chemical Engineering
National Taiwan University, Taipei 10617 Taiwan

[*]Corresponding Author's E-mail: hsiuyuyu@ntu.edu.tw

Abstract

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 phase change 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 analyze a binary-component spinodal decomposition dataset that includes transition behaviors. The data are generated using the numerical 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 the latest MAU[1] model to capture the underlying temporal and spatial correlations. With the recently developed attention and fusion mechanism, MAU can more readily capture both short and long-term memory simultaneously. In the second approach, we apply dimensional reduction processes with our newly innovated model: L-MAU, which is modified from MAU model to perform the multivariate time-series prediction. We propose two pipelines: (a) two-point correlation function combining principal component analysis (PCA) with Gerchberg-Saxton[2] algorithm, and (b) autoencoder combining PCA to accelerate the phase-field prediction. With the help of dimensionality reduction, we can reduce the heavy computational workload in the original MAU model. At the meantime, the new L-MAU model outperforms the traditional recurrent neural network in predicting multivariate low dimensional representatives.

Keywords: Phase-field model; Cahn-Hilliard equation; Machine learning; Spatiotemporal prediction

Reference

1. Chang Z, Zhang X, Wang S, Ma S, Ye Y, Xinguang X, et al. MAU: A Motion-Aware Unit for Video Prediction and Beyond. Advances in Neural Information Processing Systems. 2021;34:26950-62.
2. Fullwood DT, Niezgoda SR, Kalidindi SR. Microstructure reconstructions from 2-point statistics using phase-recovery algorithms. Acta Materialia. 2008;56(5):942-8.