Materials Science & Engineering Dissertation Defense

Novel data-driven emulator for predicting microstructure evolutions

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Abstract

Phase-field (PF) models are one of the most powerful tools to simulate microstructural evolution in metallic materials, polymers, and ceramics. However, existing PF approaches rely on rigorous mathematical model development, sophisticated numerical schemes, and high-performance computing for accuracy. Although recently developed surrogate microstructure models employ deep-learning techniques and reconstruction of microstructures from lower-dimensional data, their accuracy is fairly limited as spatiotemporal information is lost in the pursuit of dimensional reduction. Given these limitations, we present a novel data-driven emulator (DDE) for extrapolation prediction of microstructural evolution, which combines an image-based convolutional and recurrent neural network (CRNN) with tensor decomposition, while leveraging previously obtained PF datasets for training. To assess the robustness of DDE, we also compare the emulation sequence and the scaling behavior with phase-field simulations for several noisy initial states. Finally, we discuss the effectiveness of our microstructure emulation technique in the context of runtime speed-up while also highlighting its trade-off with accuracy.

Meanwhile, an interpolation DDE has also been tested, which is based on obtaining a low-dimensional representation of the microstructures via tensor decomposition and subsequently predicting the microstructure evolution in the low-dimensional space using Gaussian process regression (GPR). Once we obtain the microstructure prediction in the low-dimensional space, we employ a hybrid input-output phase retrieval algorithm to reconstruct the microstructures. As proof of concept, we present the results on microstructure prediction for spinodal decomposition, although the method itself is agnostic of the material parameters. Results show that we are able to predict microstructure evolution sequences that closely resemble the true microstructures (average normalized mean square of 6.78×10^{-7}) at time scales half of that employed in obtaining training data. Our data-driven microstructure emulator opens new avenues to predict the microstructural evolution by leveraging phase-field simulations and physical experimentation where the time resolution is often quite large due to limited resources and physical constraints, such as the phase coarsening experiments previously performed in microgravity.

Future work will also be discussed and show how we plan use these two approached to do a 3D microstructure prediction by combining these two methods.

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