MLDL

SAND2020-7003PE

Machine Learning and Deep Learning Conference 2020

Accelerating phase-field based predictions via surrogate models trained by machine learning methods

- **This template is required for all submissions, both posters and oral presentations, but does not constrain or define the final form of the presentation.**
  - **Classified presenters must submit an unclassified template AND a classified template upon request.**
- **All submissions must ≤ 10 slides.**
- **Submissions should be reviewed by a derivative classifier.**
- **Formal Review and Approval is required for all presentations at the conference.**

- **Presenter:** R. Dingreville (1881)
- **Co-presenters:** D. Montes de Oca Zapiain (1881), J.A. Stewart (2554)

- **Funding source:** LDRD, DOE BES

Abstract

The phase-field method has emerged as a powerful and versatile computational approach for modeling the coevolution of microstructure and properties in a wide variety of physical, chemical and biological systems. Existing high-fidelity phase-field models describe these evolutionary processes by solving a system of coupled partial differential equations for the evolution of continuous field variables, but such simulations are inherently computationally expensive requiring high-performance computing resources and sophisticated numerical integration schemes.

In this talk, I will discuss how to bypass these difficulties by directly learning the microstructure evolution via a computationally inexpensive and accurate, data-driven surrogate model combining phase-field and deep learning techniques. I will explain how to construct this surrogate model by combining a statistically-representative, low-dimensional representation of the microstructure obtained directly from phase-field simulations with either a Time-Series Multivariate Adaptive Regression Splines (TSMARS) autoregressive algorithm or a Long Short-Term Memory (LSTM) network. I will then go over our results to discuss the accuracy and computational efficiency of our machine-learned surrogate model to predict the non-linear microstructure evolution during the spinodal decomposition of a two-phase mixture using modest computational resources and without the need for ``on-the-fly" solutions of the phase-field equations-of-motion. I will finally conclude this talk with some thoughts on opportunities such machine-learned model offer to discover and design new materials.

Problem you are trying to solve

- Existing high-fidelity mesoscale phase-field models are inherently computationally expensive because they solve a system of coupled partial differential equations for a set of continuous field variables that describe these processes.

$$F = \int \left[f(\boxed{\eta_1, \ldots, \eta_p}, \boxed{c_1, \ldots, c_n}) + \sum_{i=1}^{n} \alpha_i (\nabla c_i)^2 + \sum_{j}^{3} \sum_{k}^{p} \beta_{ij} \nabla_i \eta_k \nabla_j \eta_k \right] d\Omega$$

Allen-Cahn:
Non-conserved

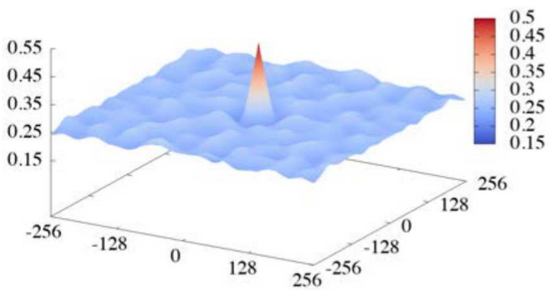
$$\frac{\partial \eta_p}{\partial t} = -M_{pq} \frac{\delta F}{\delta \eta_q}$$

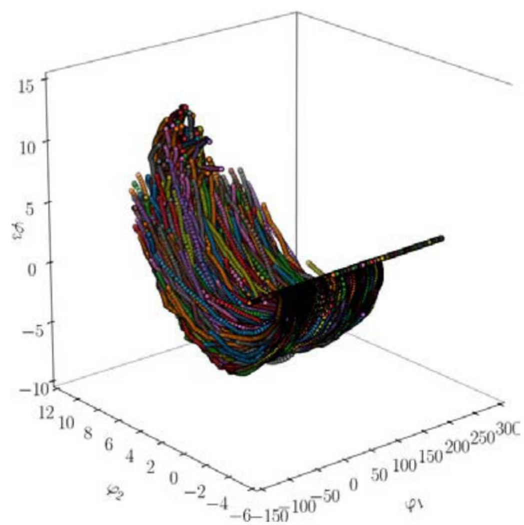
Cahn-Hillard:
Conserved

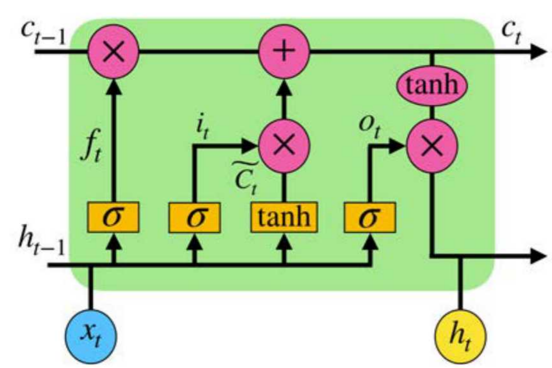
$$\frac{\partial c_i}{\partial t} = \nabla \left(M_{ij} \frac{\delta F}{\delta c_j} \right)$$

Algorithmic approach of your solution

- We reframe phase-field simulations as a multivariate time series problem forecasting the microstructure evolution in a low-dimensional representation:
  - At equally spaced interval during the phase-field simulation, we first calculate the microstructure 2pt. spatial autocorrelation to obtain a statistically representative quantification of the microstructure
  - We reduce the dimensionality via principal component analysis (PCA)
  - We exploit the time-history of the PCA representation to predict the microstructure evolution via TSMARS or LSTM
  - Predictions from machine-learned surrogate can be used as input in a classical phase-field simulation

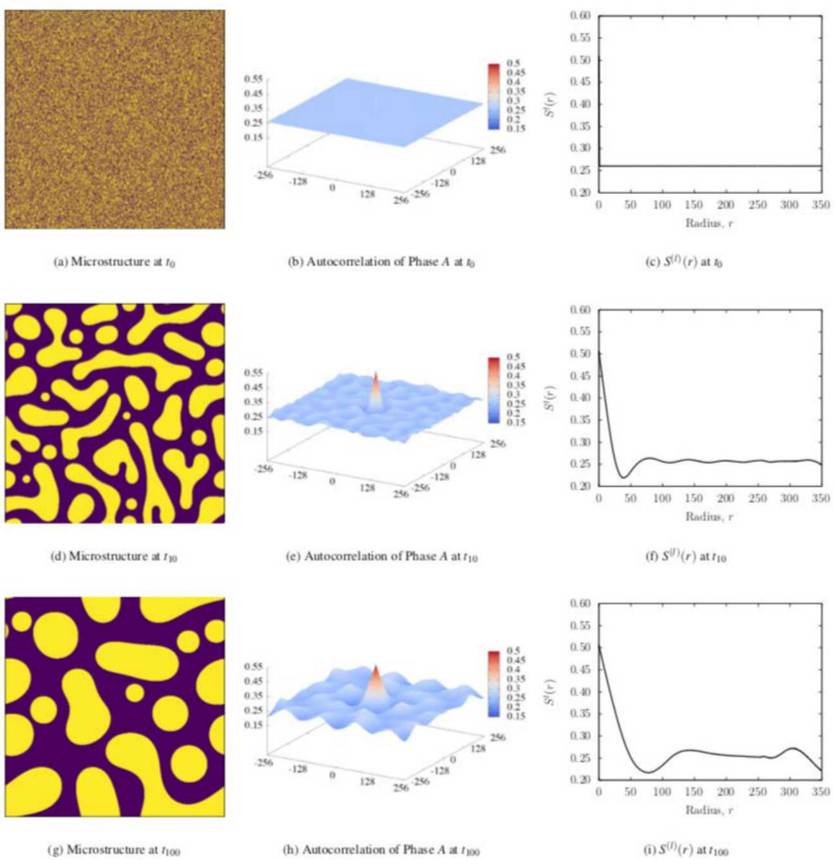


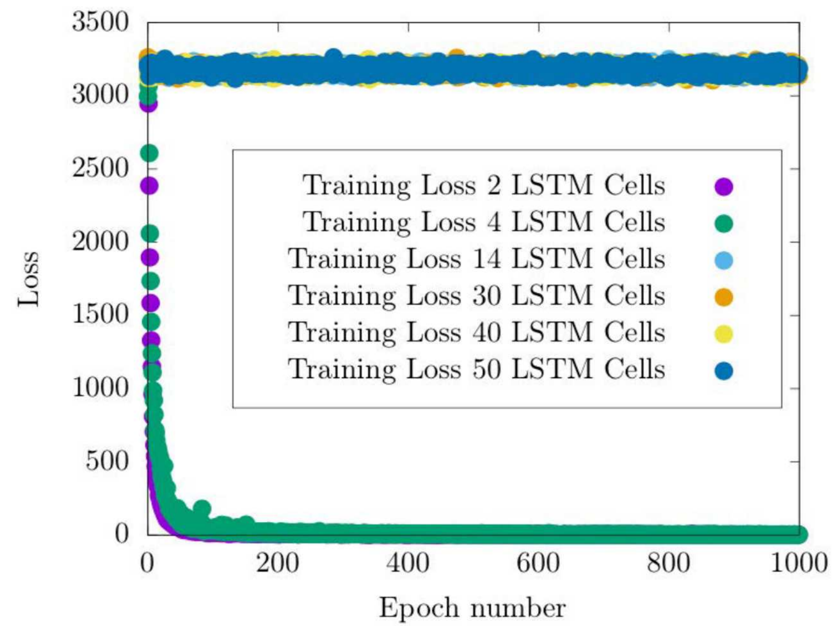




Description of the data used

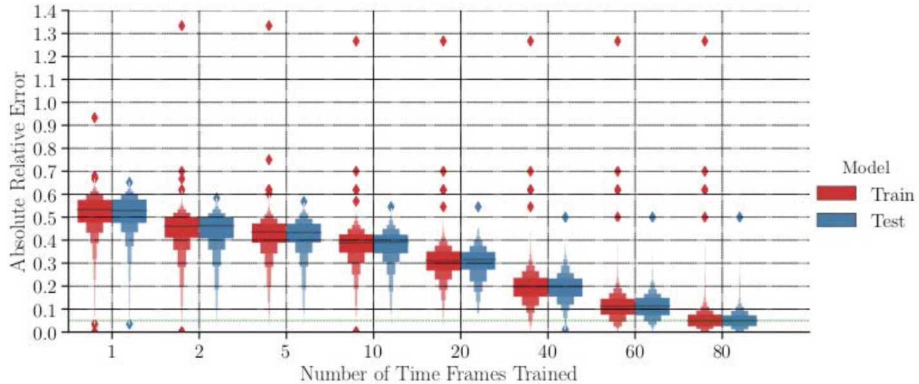
- We use our in-house multi-physics phase-field code MEMPHIS to generate 5500 history-dependent microstructure evolution trajectories.
- 5,000 simulations are used as training data
- 500 simulations are used as testing data

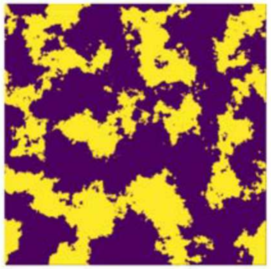




Results

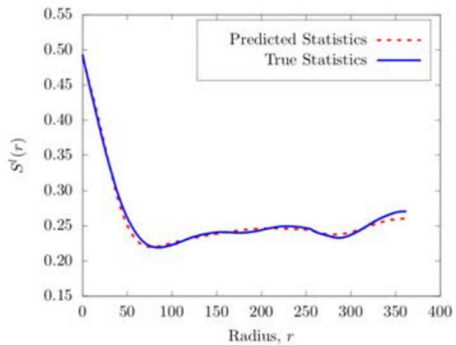
- LSTM neural network was chosen as. The primary machine-learning architecture to accelerate phase-field predictions
- LSTM-based surrogate model yields better accuracy and long-term predictability since it accounts for entire history of microstructure evolution
- Predictions of microstructure evolutions are performance in a fraction of a second





(a) Microstructure Reconstructed using Phase Recovery Algorithm at t_{95}

(b) Accelerated Phase-field Resultant Microstructure



Radial Average

Conclusions

Indicate at which session you'd like to present

Unclassified Machine Learning Day or Deep Learning Day

What is the one-sentence summary of your work that you would want a technical person to remember?

Our machine-learned phase-field framework accurately predicts the non-linear microstructure evolution in a fraction of a second (as opposed to hours) by utilizing a history-dependent machine learning approach to exploit information from the time-history of a low-dimensional representation of the microstructure.

What is the one-sentence summary of your work that you would want a manager or program developer to remember?

Our machine-learned mesoscale phase-field framework opens a promising path forward to novel uses of predictive modeling algorithms for discovering, understanding, and predicting processing-microstructure-performance relationships relevant to SNL mission.

Do you prefer an oral or a poster presentation?

Oral

If oral, indicate presentation time between 15 and 30 minutes or a 5-minute spotlight.

15 or 20 mins.