Accelerated Microstructure Evolution Predictions Using Machine Learning Based Reduced-Order Models

David Montes de Oca Zapiain[1,2], James A. Stewart[1,2], Remi Dingreville[1,2]
[1]*Sandia National Laboratories, Albuquerque, NM 87185, USA*
[2]*Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM 87185, USA*

SAND2019-15266C

U.S. DEPARTMENT OF ENERGY
Office of Science

Executive Summary

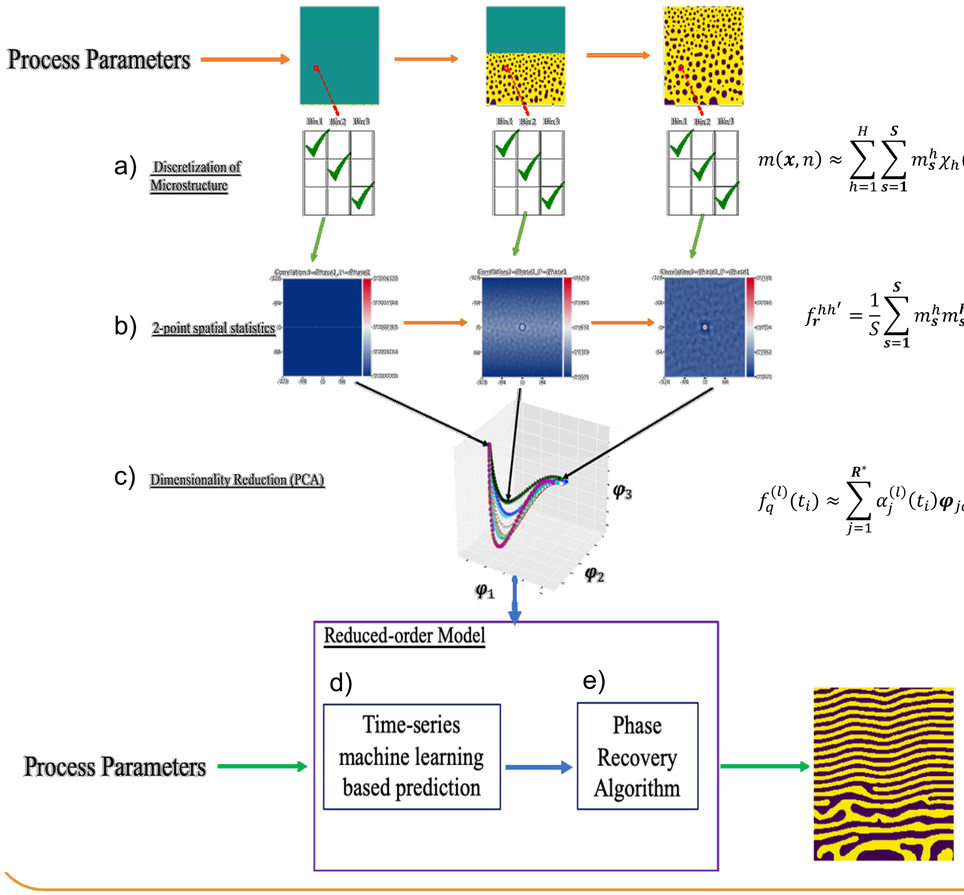
Problem: The numerical nature of phase-field models causes for these model to be ill-suited for scenarios where a large number of candidate microstructures need to be evaluated to identify an optimal solution (i.e., inverse-type problems and high-throughput scenarios).

Solution: We developed high-fidelity surrogate mesoscale models that accurately predict microstructure evolution without the need to numerically solve the computationally intensive phase-field equations. This is achieved by combining low-dimensional statistically representative microstructure representation with machine learning and time-series analysis techniques.

Results: The protocol developed in this work successfully established a reduced-order model that accurately predicts the microstructure evolution with a significantly reduced computational load: our simulations only **required 5 minutes on a regular laptop** while the explicit phase field model simulations **required 90 minutes on 180 processors**.

Conclusions: The ability to obtain accurate yet fast phase-field-based microstructure evolution results will enable unbiased automated explorations of vast model spaces to identify the optimal process and material parameters for any desired evolutionary process.

Protocol for Establishing the Reduced-Order Model



$$m(\boldsymbol{x},n) \approx \sum_{h=1}^{H}\sum_{s=1}^{S} m_s^h \chi_h(n)\chi_s(\boldsymbol{x})$$

$$f_r^{hh'} = \frac{1}{S}\sum_{s=1}^{S} m_s^h m_{s+r}^{h'}$$

$$f_q^{(l)}(t_i) \approx \sum_{j=1}^{R^*} \alpha_j^{(l)}(t_i)\boldsymbol{\varphi}_{jq} + \tilde{f}_q$$

a) The microstructure of the material is quantified using digital representation of the microstructure [1].

b) 2-point spatial correlations are calculated on this digital representation in order to obtain a statistical representation of the microstructure [1].

c) Principal Component Aanalysis (PCA) enables us to obtain an objective (data-driven) low-dimensional representation of the defined statistical description of the microstructure [1].

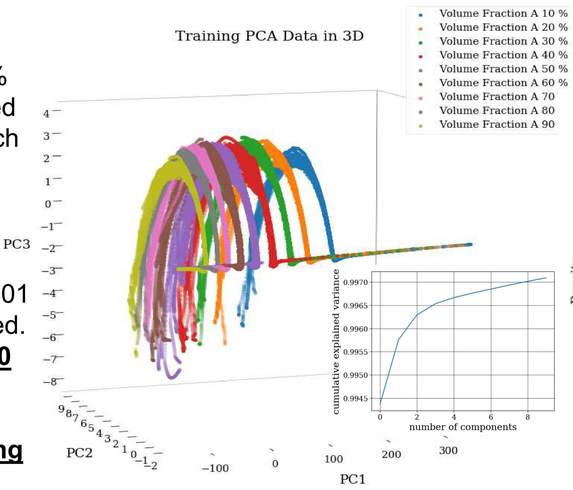
d) Time Series Multivariate Adaptive Regression Splines (TSMARS) [2] are used to establish a functional dependence predicting the future values of a PC components (i.e., in reduced space) based on its previous values and the process parameters. Subsequently, the predicted PC components are used to recover the spatial correlations of the structure.

e) A phase recovery algorithm [3] is used to recover the microstructure from the predicted 2-point statistics.

Case Study: Spinodal Decomposition

Building Reduced-Order Model for Spinodal Decomposition:

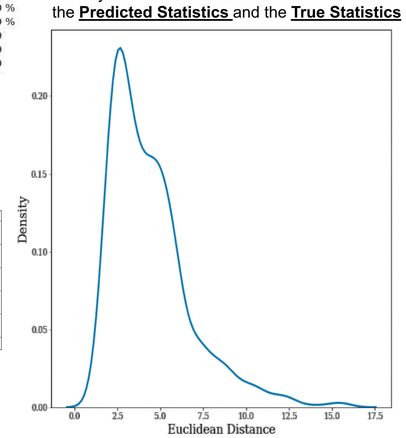
- 9 different volume fractions, sampled every 10%
- 100 Latin hypercube sampled mobilities sampled over 4 orders of magnitudes → [.01,100] for each volume fraction sampledl
- Each sampled mobility and volume fraction combination was run for 50,000,000 timesteps and 100 "snapshots" (or timesteps) of the evolution of the microstructure per simulation (101 including the initial microstructure) were captured.
- **Each simulation required 90 minutes and 180 processors.**
- Total of 900 simulations.
- **Trained the TSMARS surrogate model starting at timestep 50 for 40 timesteps.**



Training Set Results:

Predictions at timestep 100

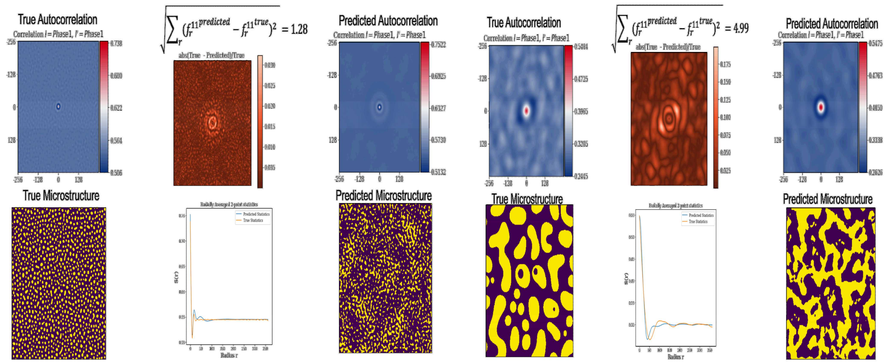
Density Plot of the Euclidean Distance between the **Predicted Statistics** and the **True Statistics**



Examples:

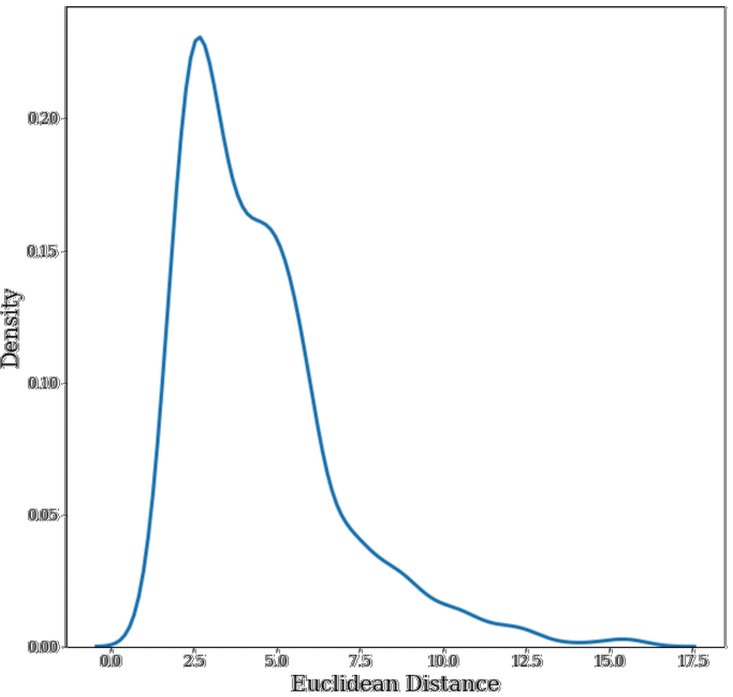
a) Initial Values:
$V_{f_A} = 10\%\ V_{f_B} = 90\%\ mob_A = .027\ mob_B = .029$

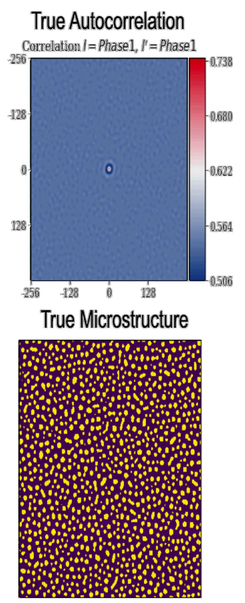
b) Initial Values:
$V_{f_A} = 40\%\ V_{f_B} = 60\%\ mob_A = .021\ mob_B = 7.39$

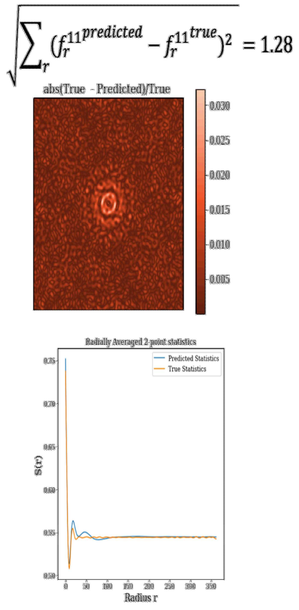


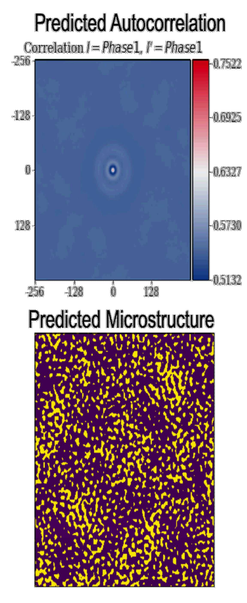
[1] Surya R Kalidindi. Hierarchical materials informatics: novel analytics for materials data. Elsevier, 2015. doi: 10.1016/ C2012- 0- 07337- 1.
[2] Jerome H Friedman et al. Multivariate adaptive regression splines. The annals of statistics, 19(1):1{67, 1991. doi:110.1214/aos/1176347963.
[3] David T Fullwood, Stephen R Niezgoda, and Surya R Kalidindi. Microstructure reconstructions from 2-point statistics using phase-recovery algorithms. Acta Materialia, 56(5):942{948, 2008. doi: 10.1016/j.actamat.2007.10.044.

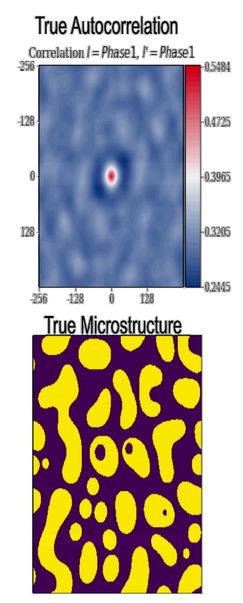
This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.

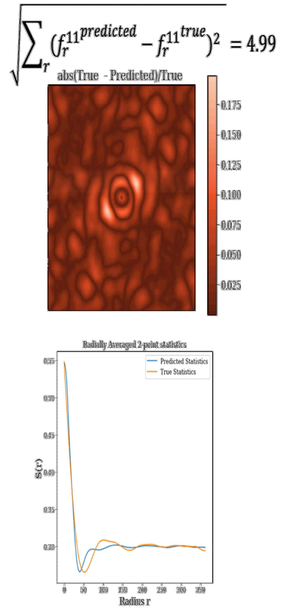

Density
0.20
0.15
0.10
0.05
0.00
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Euclidean Distance

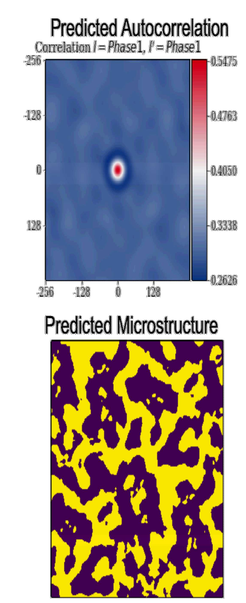

True Autocorrelation
Correlation l = Phase1, l' = Phase1
True Microstructure


$\sqrt{\sum_r (f_r^{11^{predicted}} - f_r^{11^{true}})^2} = 1.28$
abs(True - Predicted)/True
Radially Averaged 2-point statistics
Predicted Statistics
True Statistics
S(r)
Radius r


Predicted Autocorrelation
Correlation l = Phase1, l' = Phase1
Predicted Microstructure


True Autocorrelation
Correlation l = Phase1, l' = Phase1
True Microstructure


$\sqrt{\sum_r (f_r^{11^{predicted}} - f_r^{11^{true}})^2} = 4.99$
abs(True - Predicted)/True
Radially Averaged 2-point statistics
Predicted Statistics
True Statistics
S(r)
Radius r


Predicted Autocorrelation
Correlation l = Phase1, l' = Phase1
Predicted Microstructure