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Accelerating Phase-field Based Predictions Via Surrogate Models Trained by Machine Learning Methods

PRESENTED BY

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New Mexico Machine Learning Symposium

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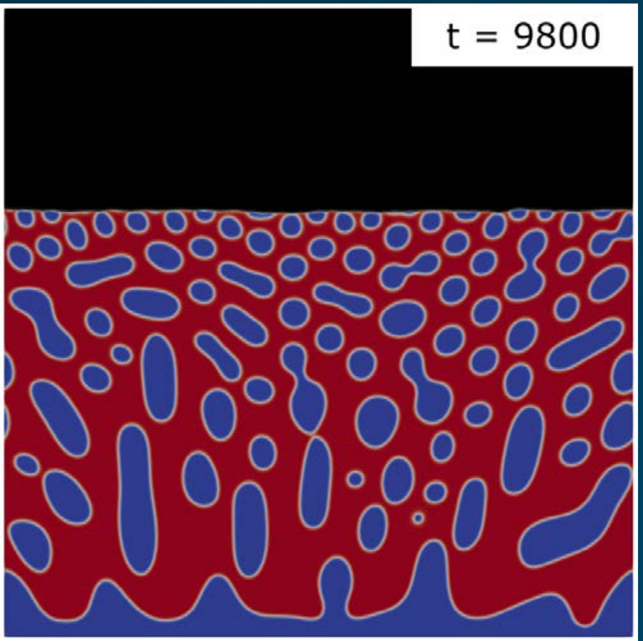
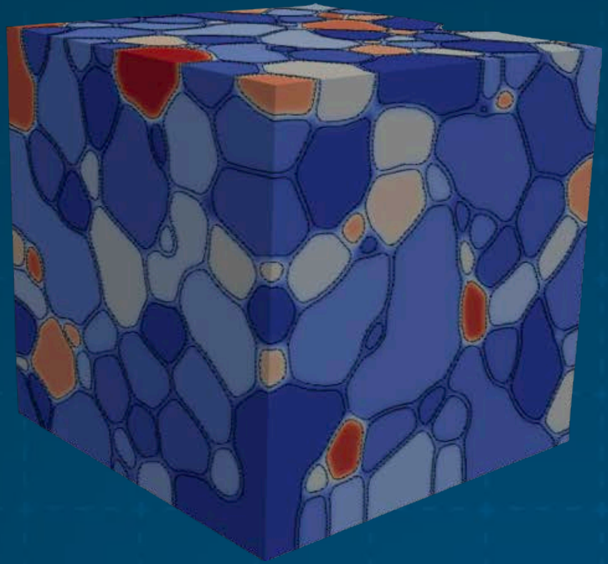
40,000 FASTER…
3 mins
0.5 s
50 mins

PREDICTING THE EVOLUTION OF MICROSTUCTURES

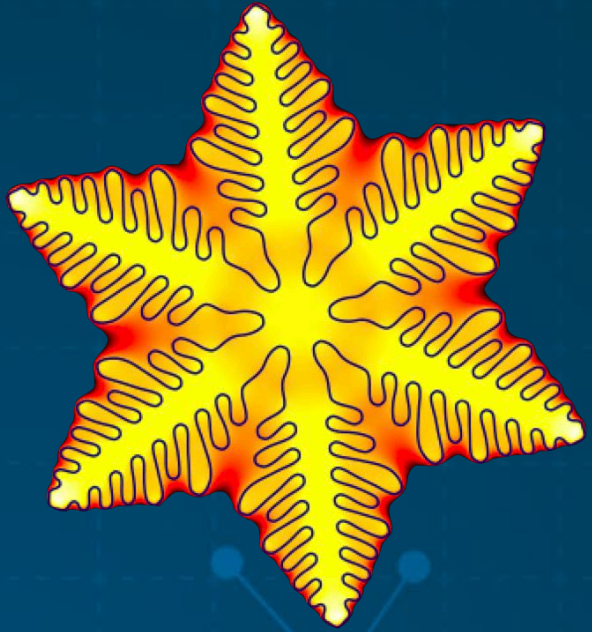
Thin-film deposition



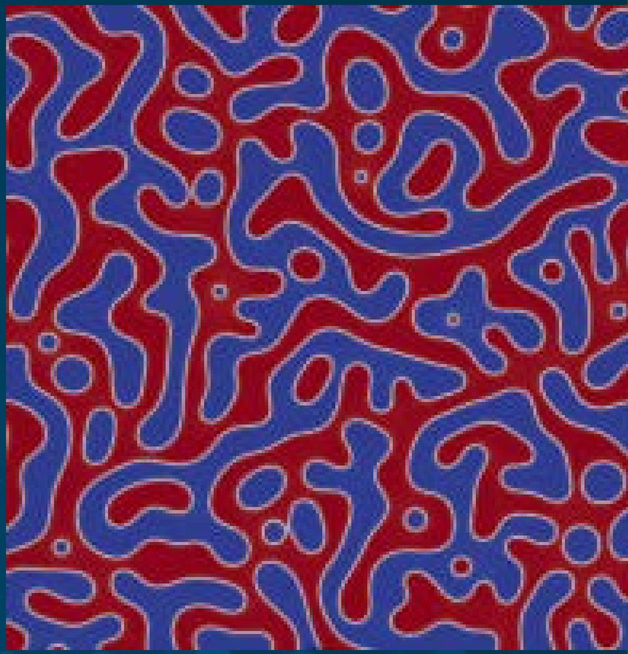
Grain growth



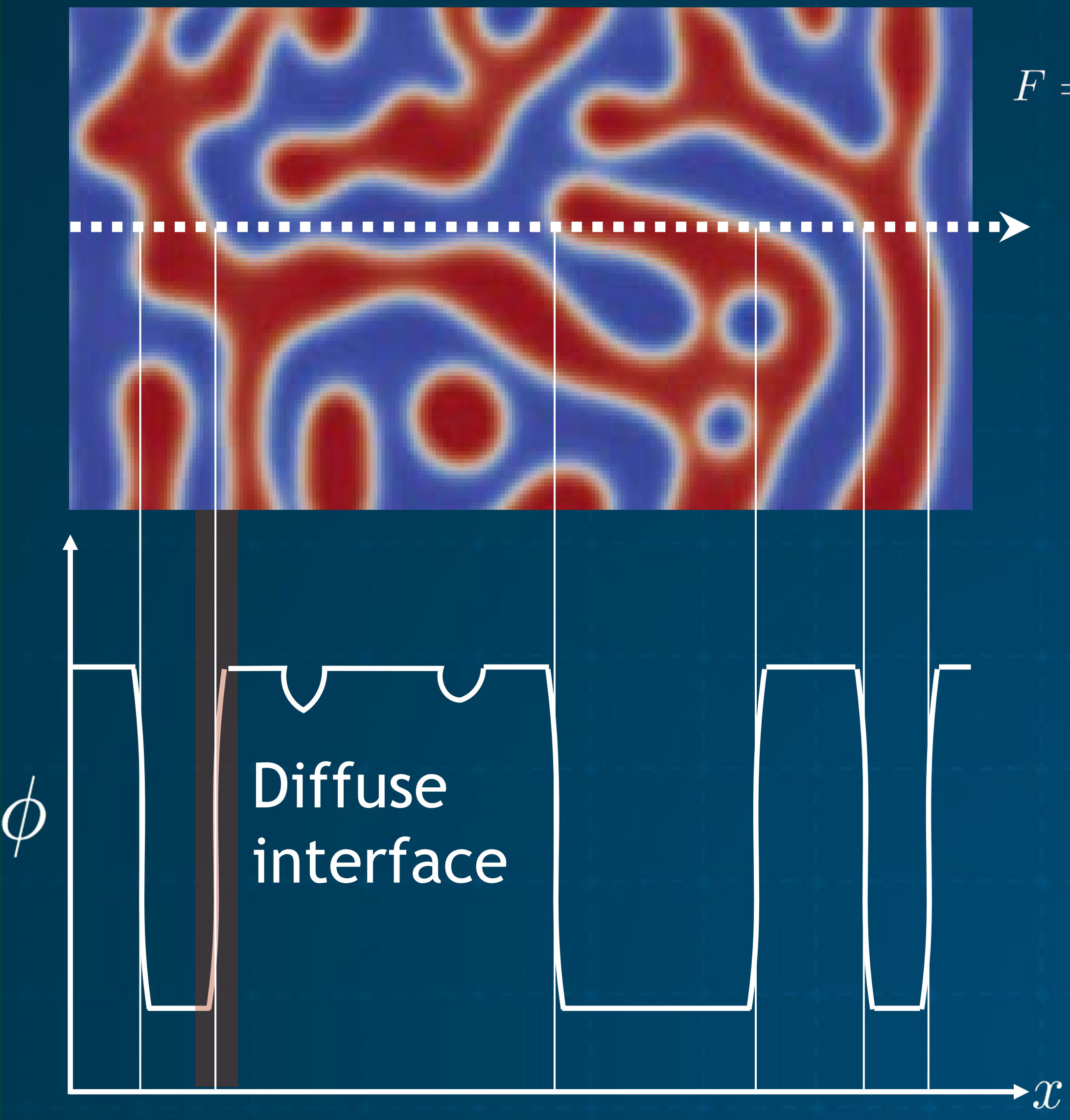
Solidification



Phase separation



Phase Field 101



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

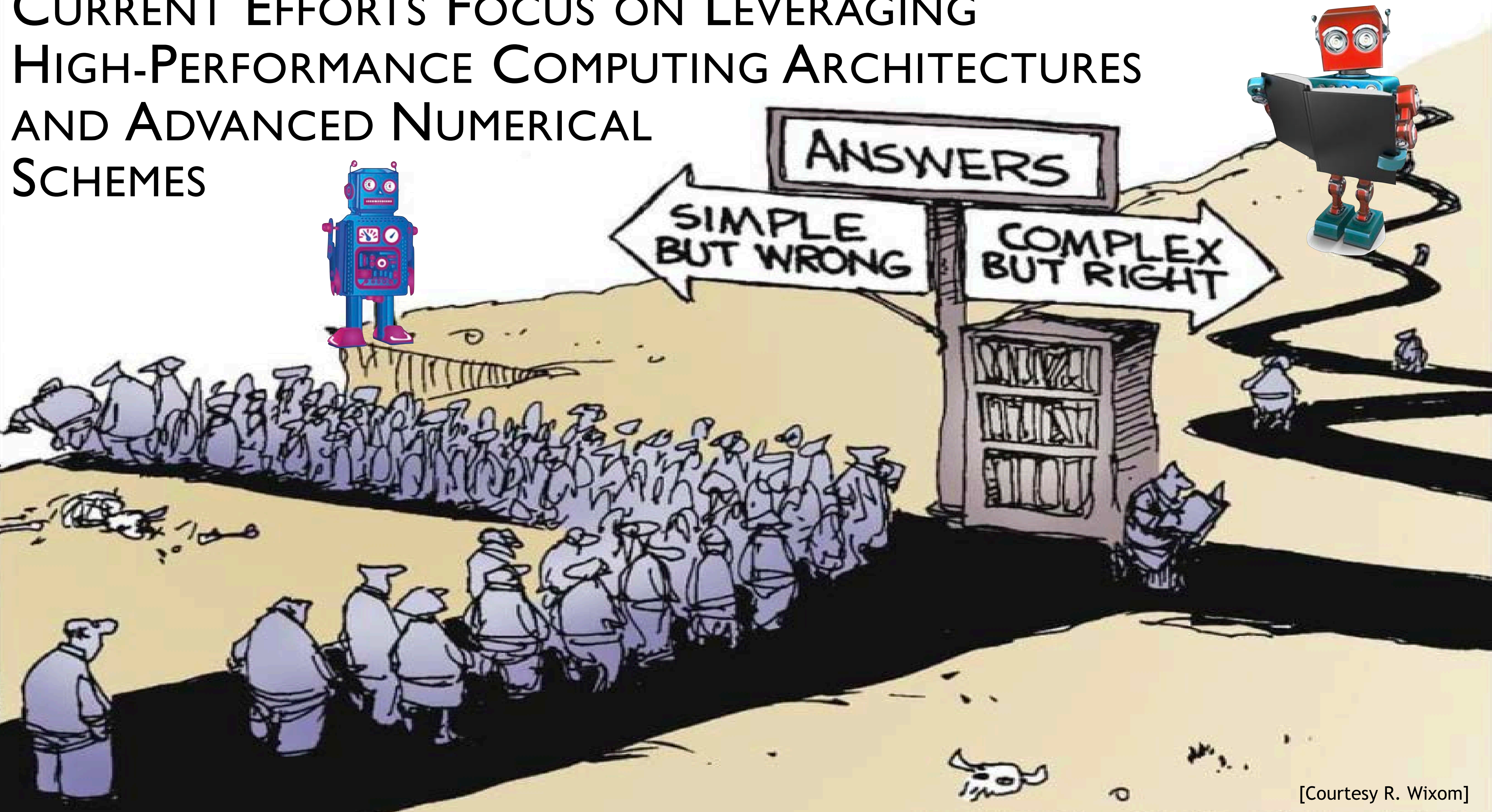
Allen-Cahn: Non-conserved

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

Cahn-Hillard: Conserved

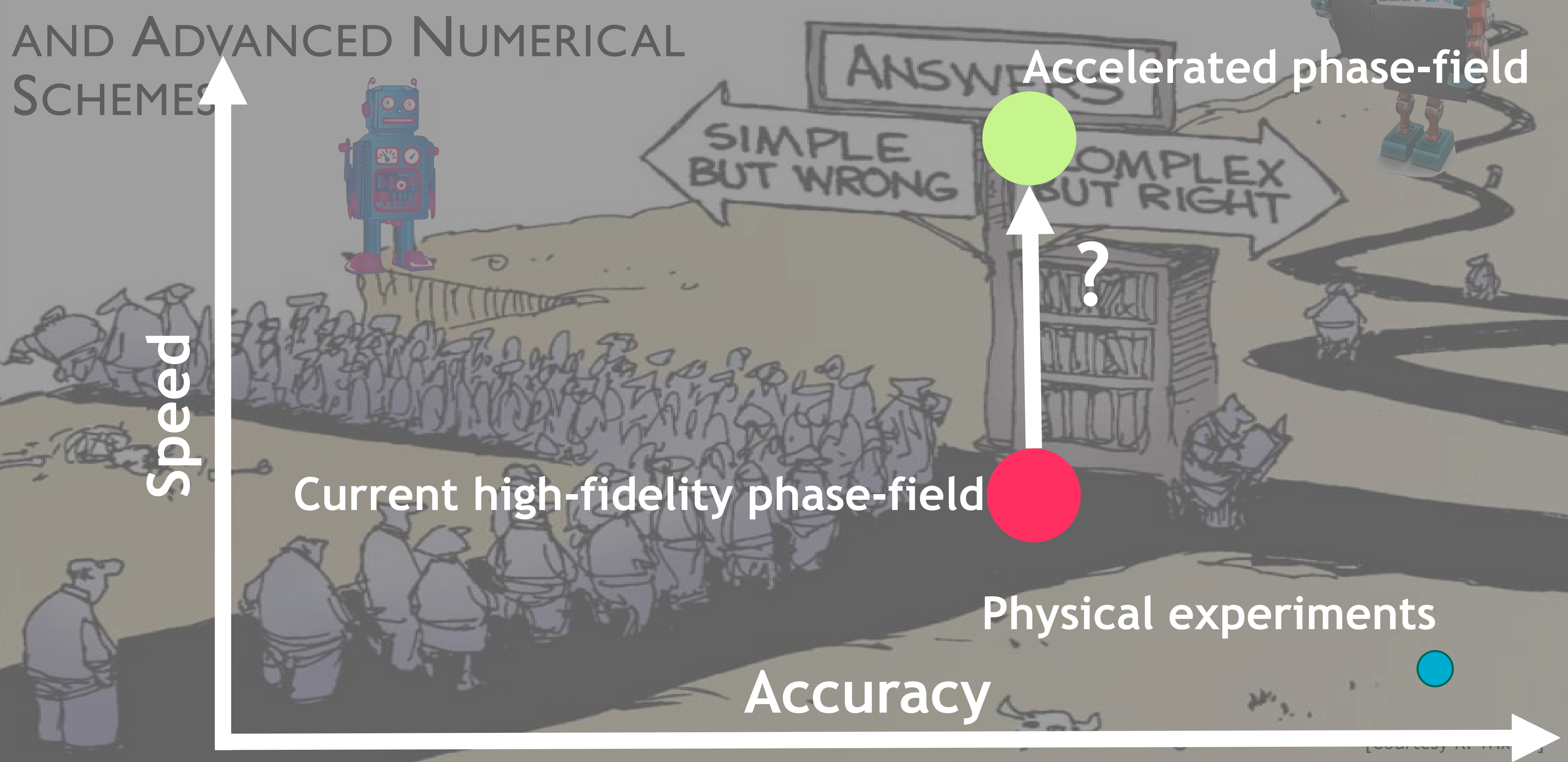
$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left(M_{ij} \nabla \frac{\delta F}{\delta c_j} \right)$$

Current Efforts Focus on Leveraging High-Performance Computing Architectures and Advanced Numerical Schemes

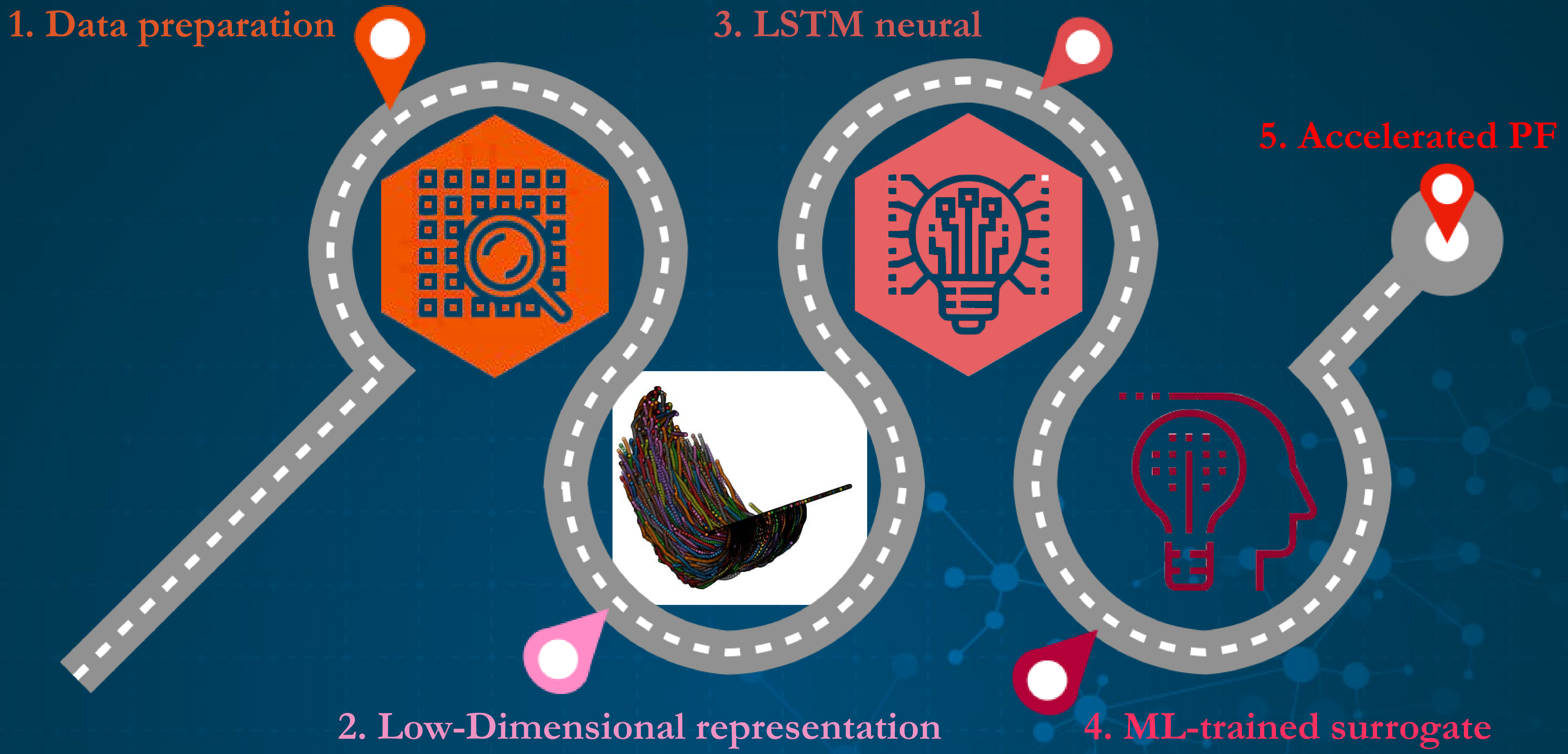


[Courtesy R. Wixom]

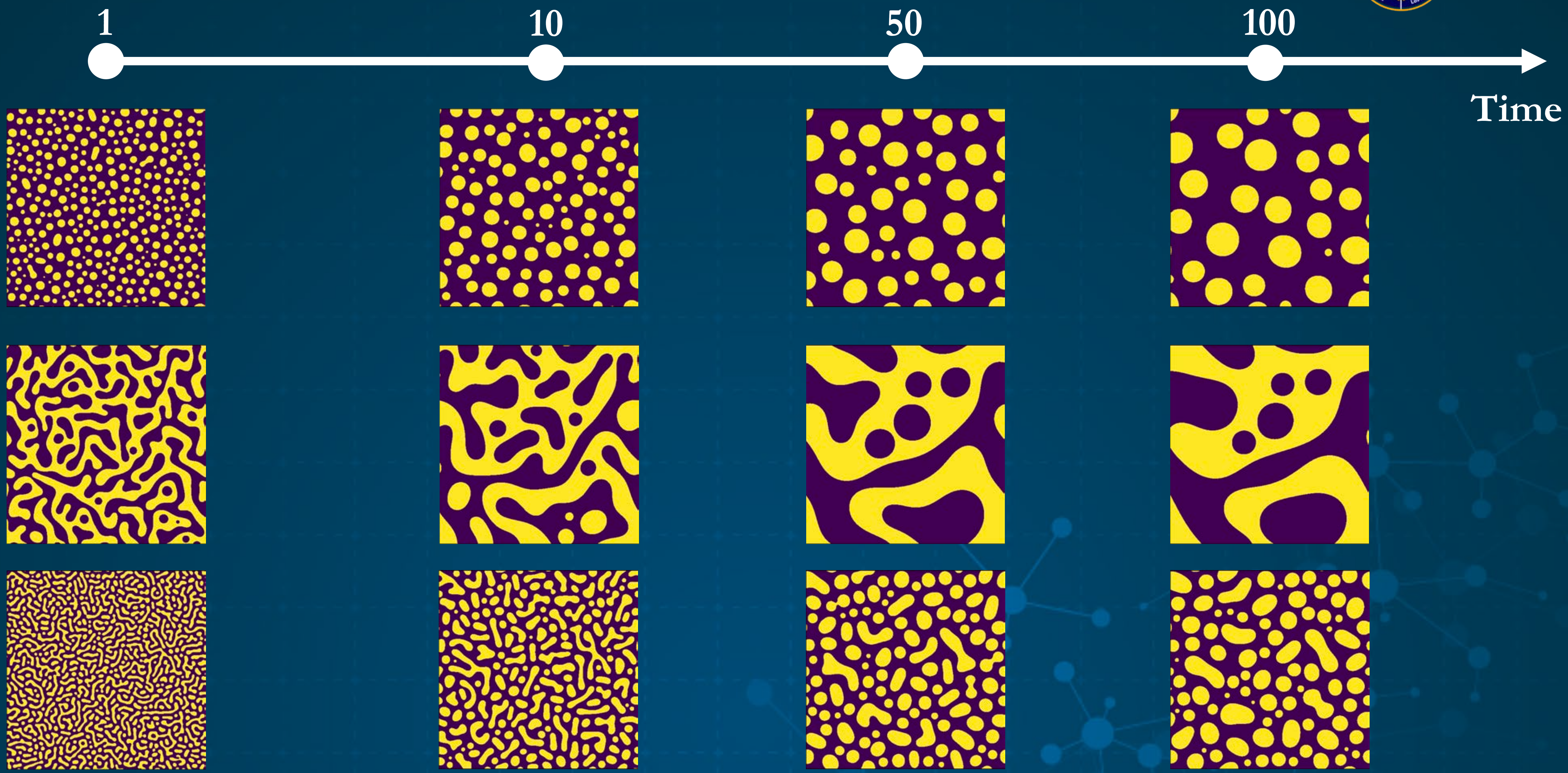
Current Efforts Focus on Leveraging High-Performance Computing Architectures and Advanced Numerical Schemes



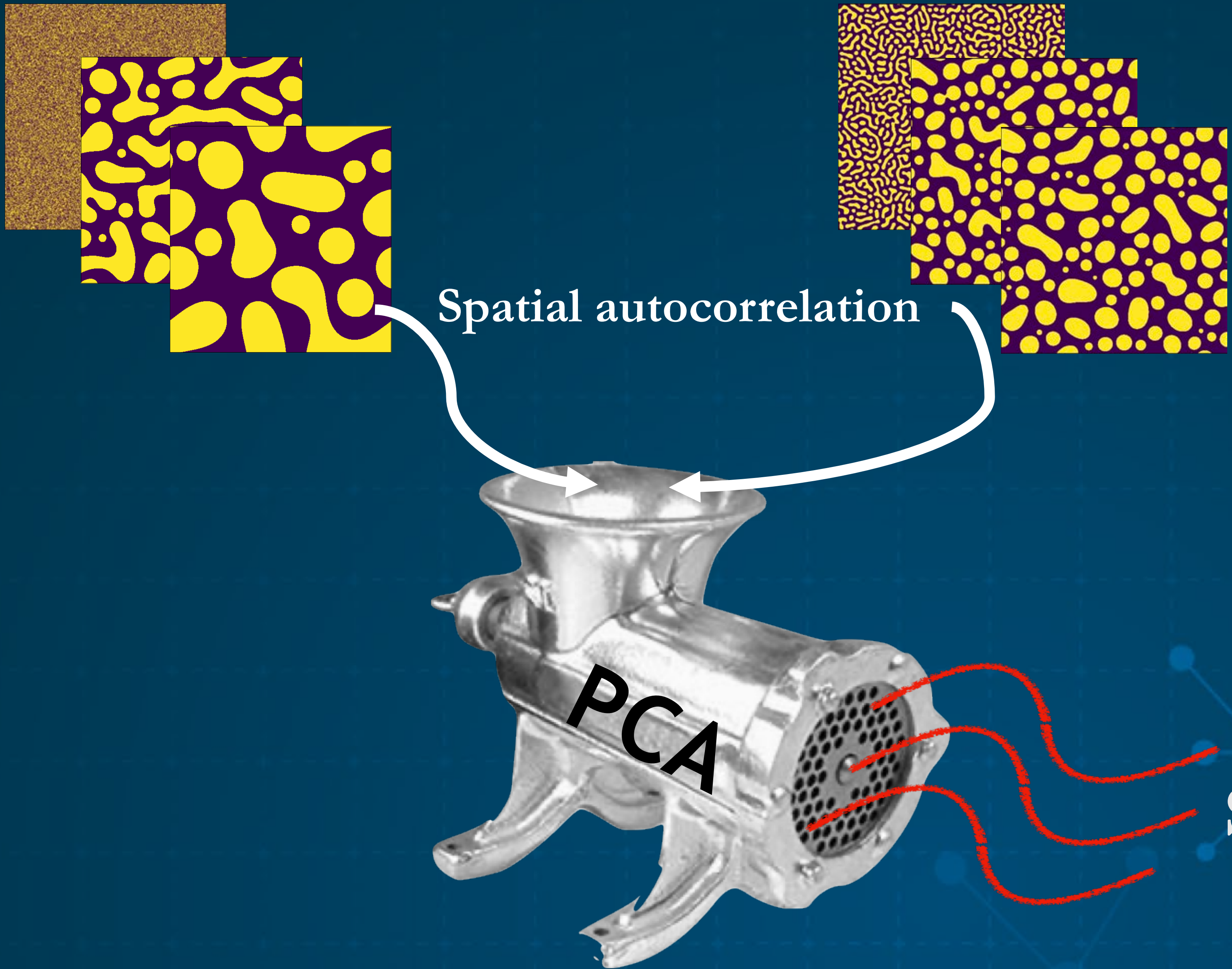
Reframing the Microstructure Evolution as a Multivariate Time-series Problem



Step 1: Data, Data, and More Data

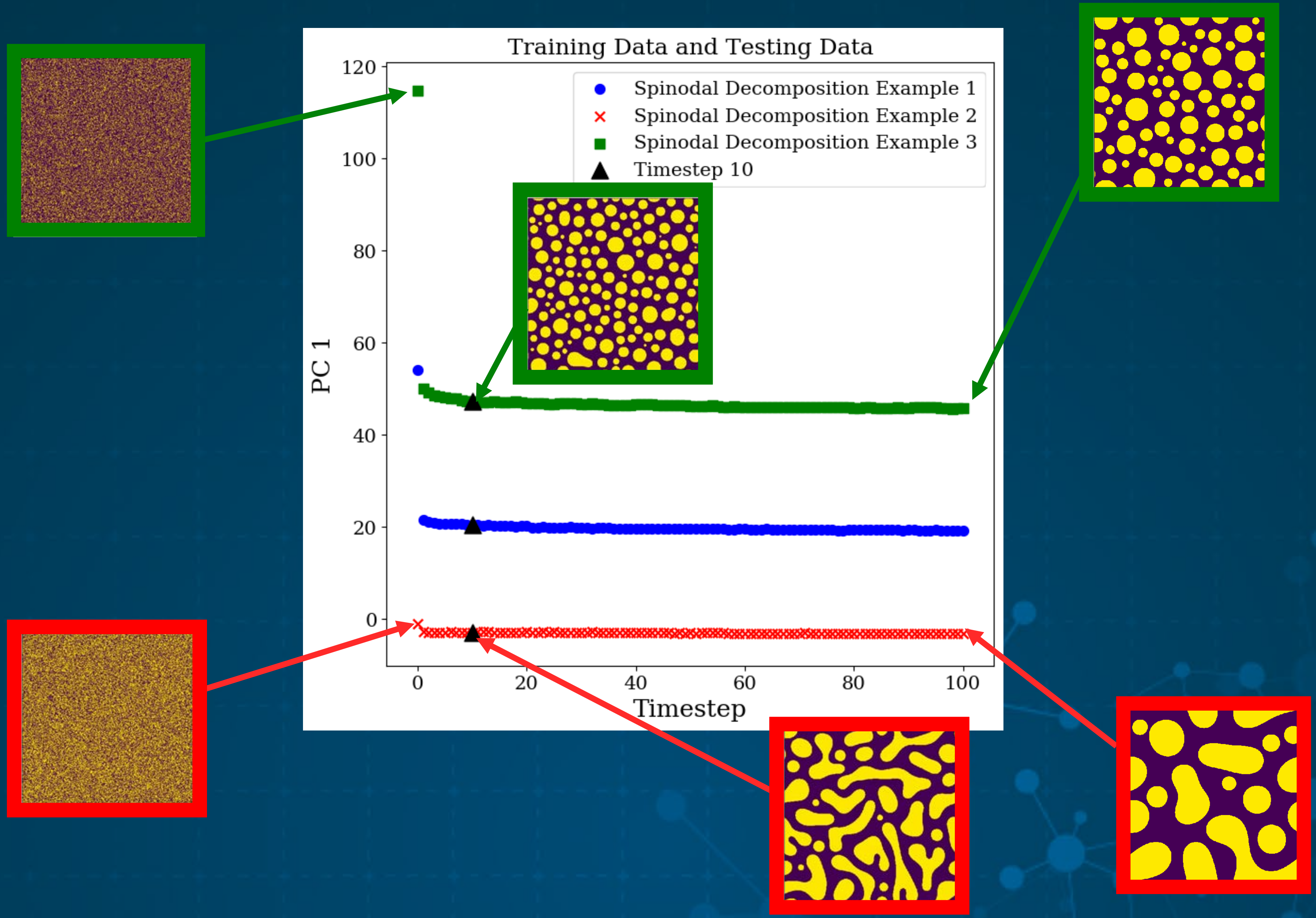


Step 2: Dimensionality Reduction

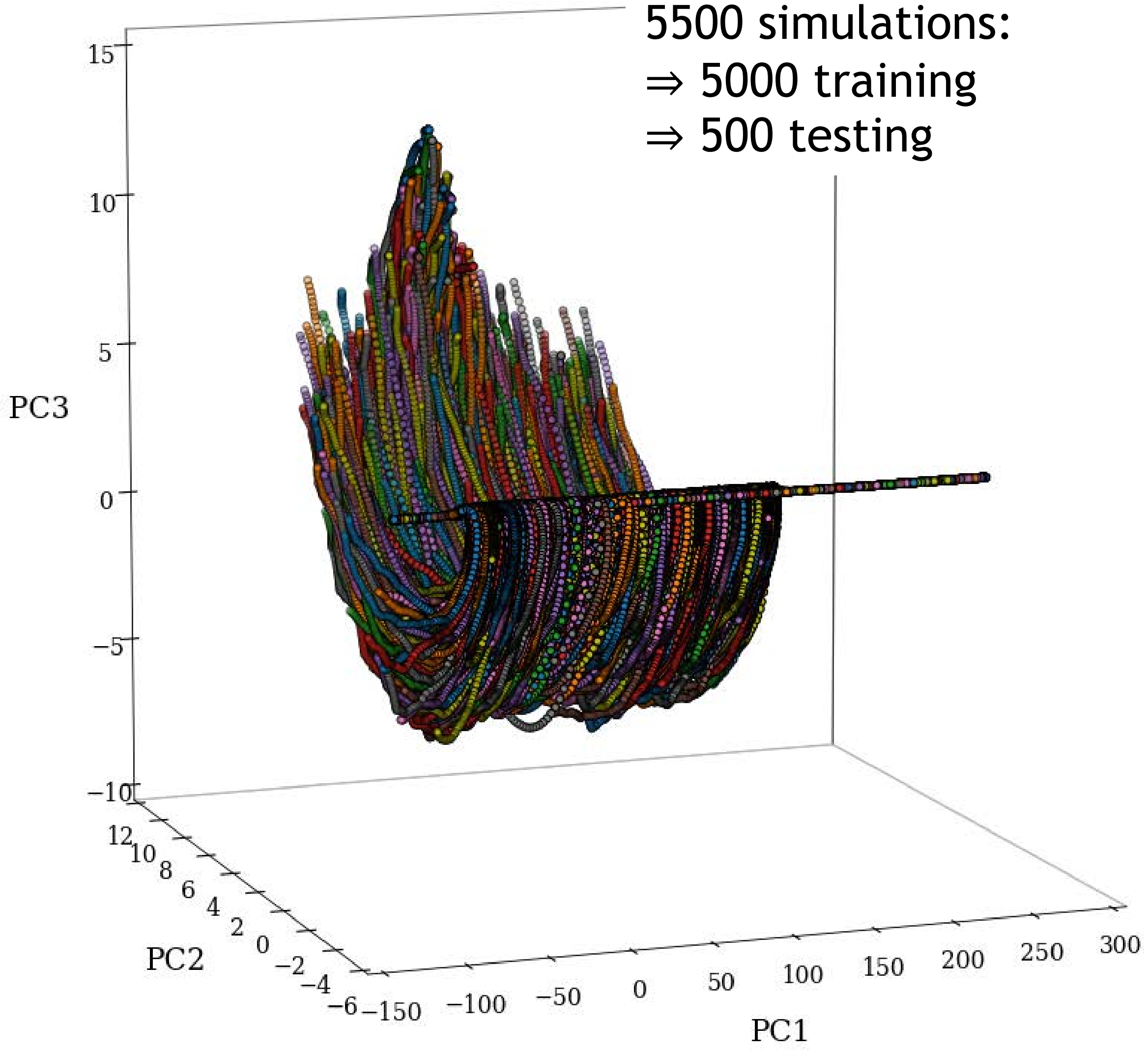


$$\mathbf{S}_{\text{pca}}^{(k)} = \sum_{j=1}^{Q} \alpha_j^{(k)}(t_i)\varphi_j + \bar{\mathbf{S}}$$

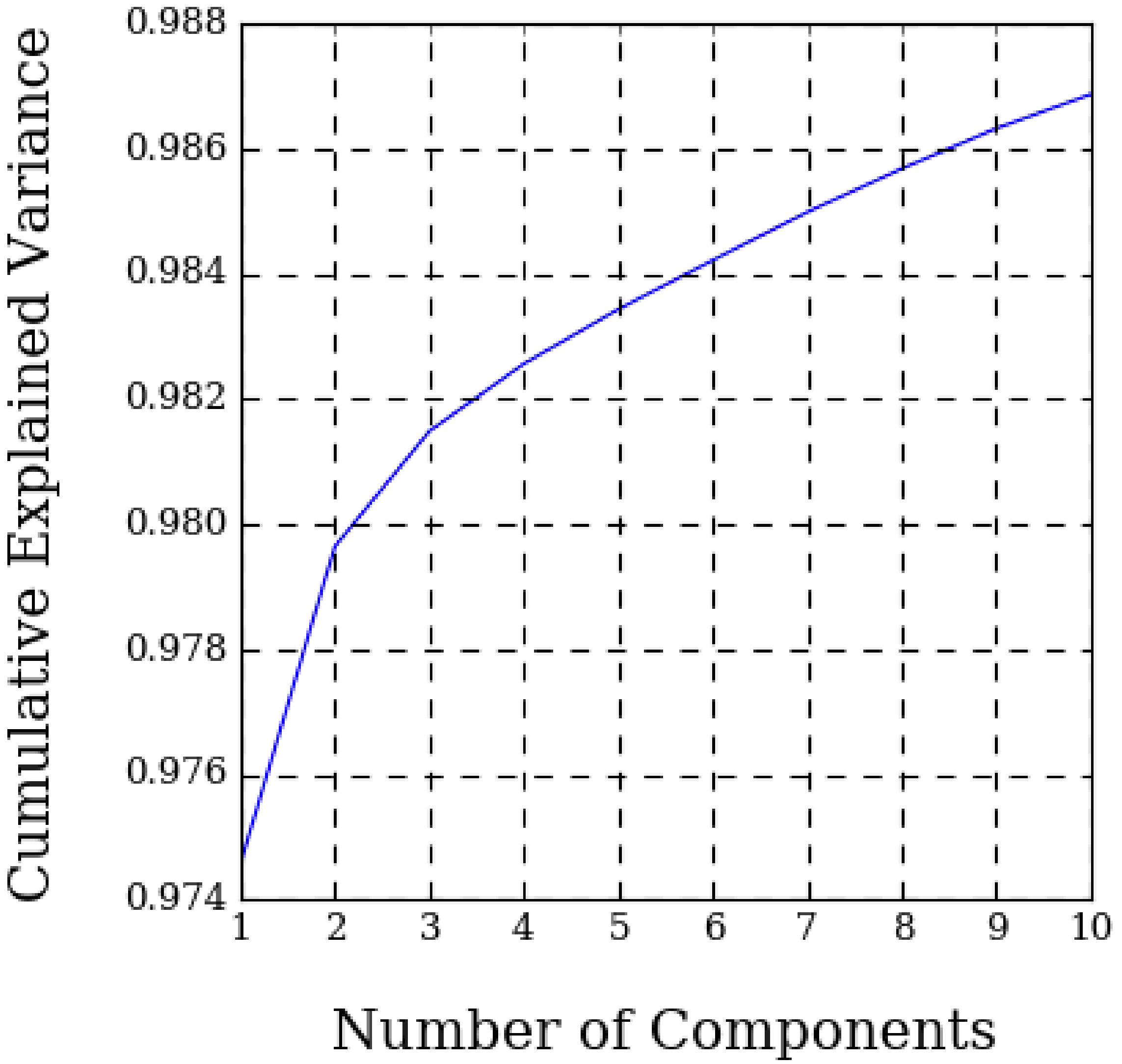
Microstructure Trajectory in Reduced Space



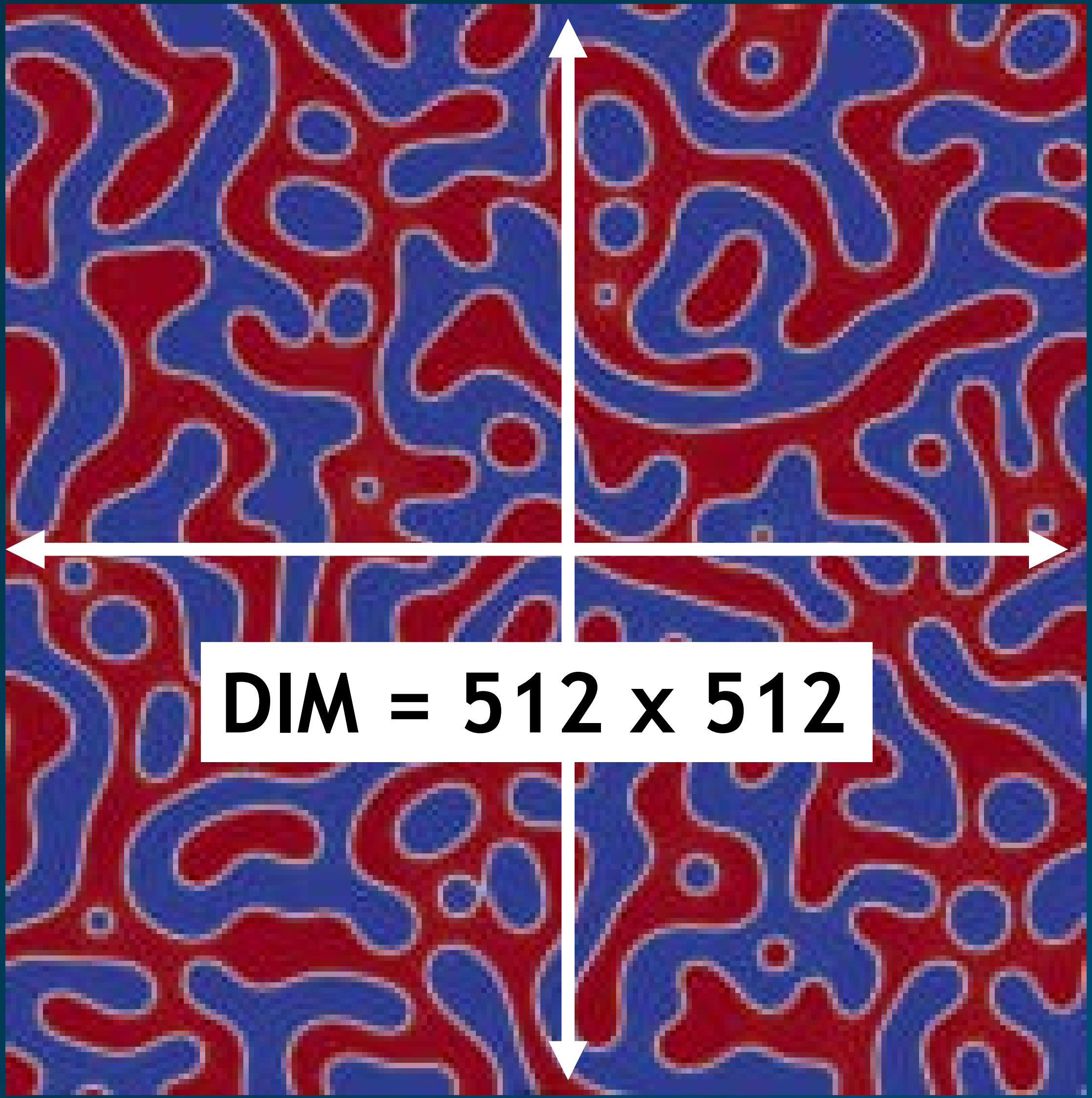
MICROSTRUCTURE TRAJECTORY IN REDUCED SPACE

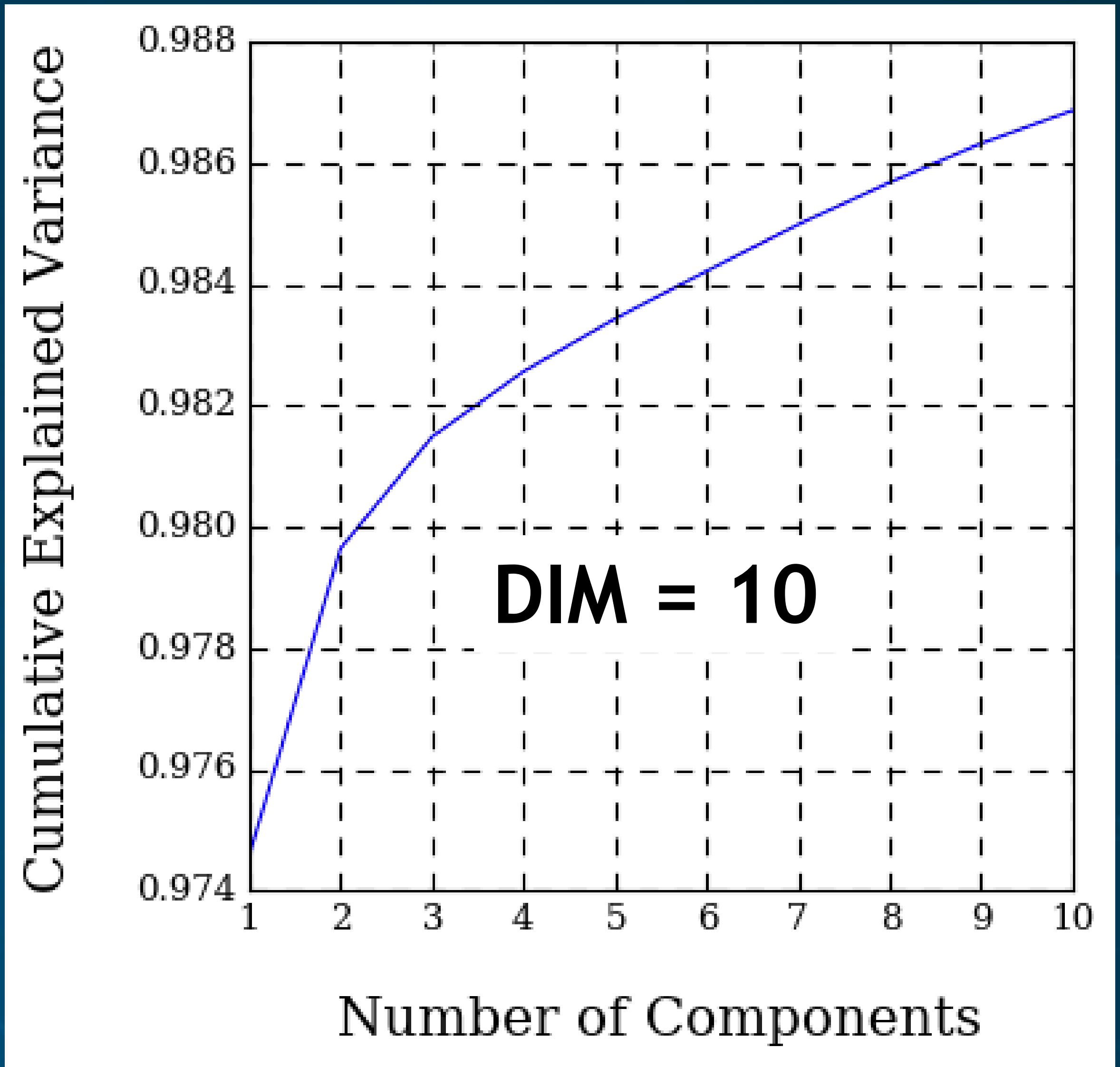


5500 simulations:
⇒ 5000 training
⇒ 500 testing



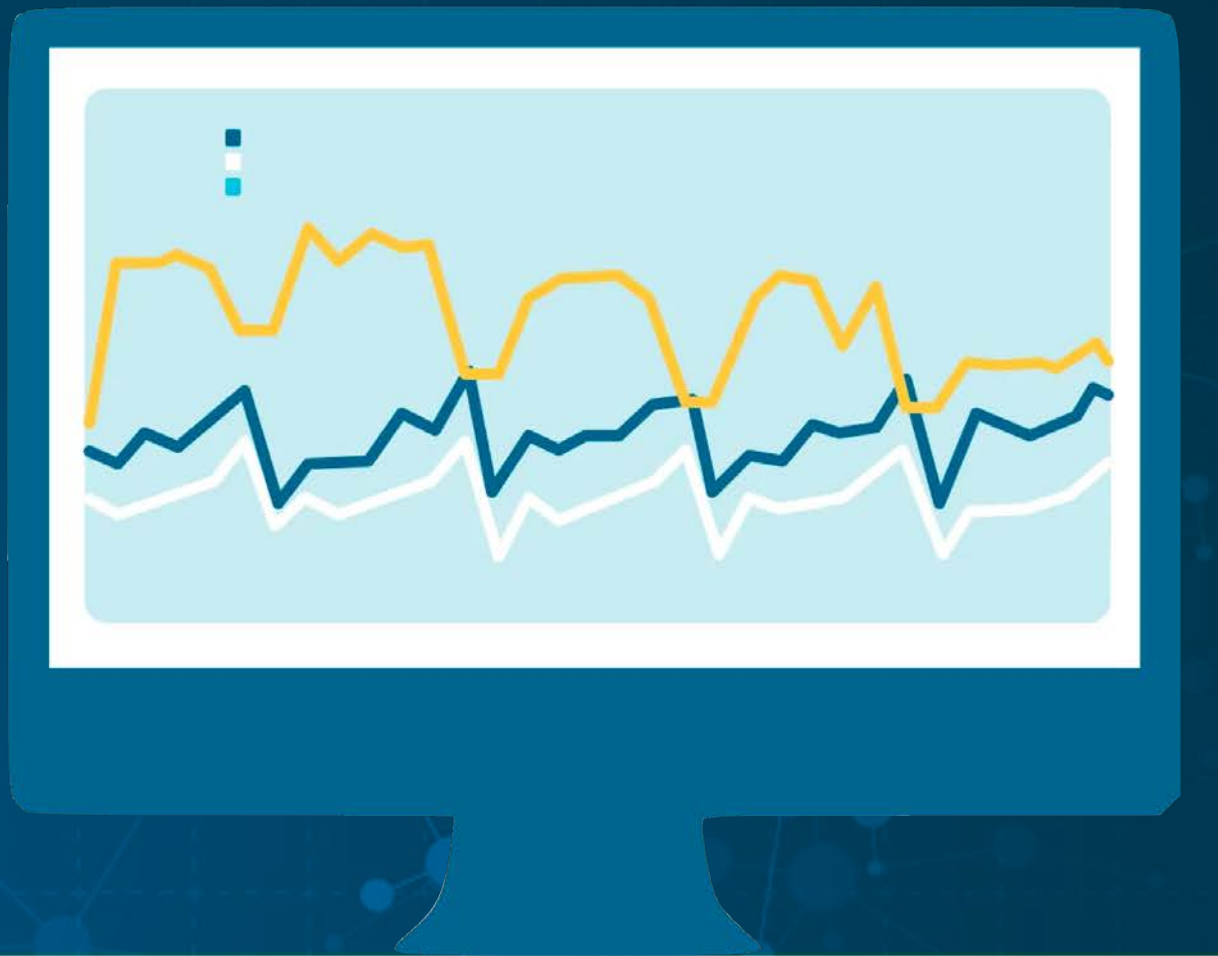
Reducing the Dimensionality by a Factor of 26,000



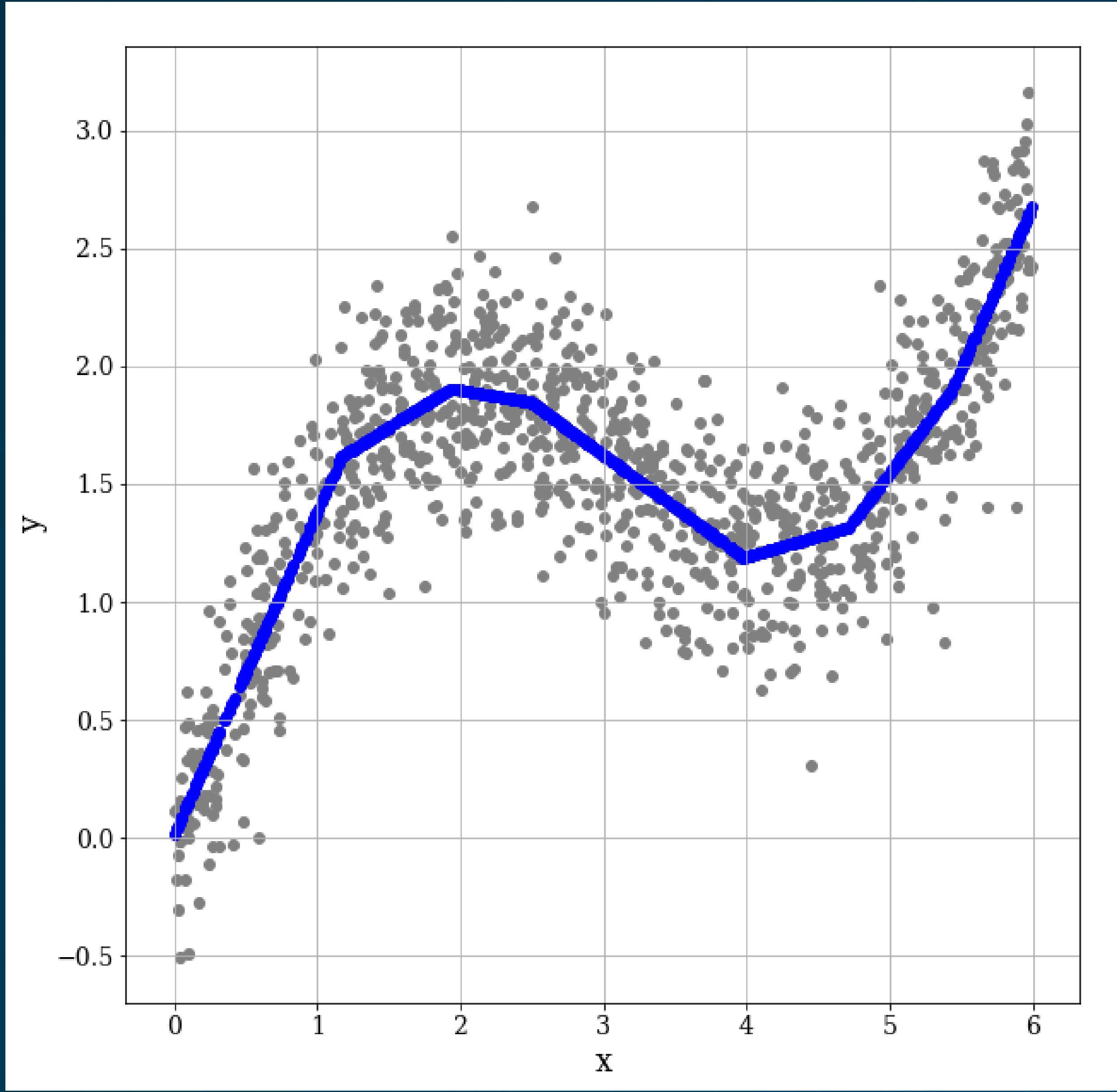


Step 3: Time-series Forecasting

Now the problem reduces to predicting the microstructure evolution in reduced space



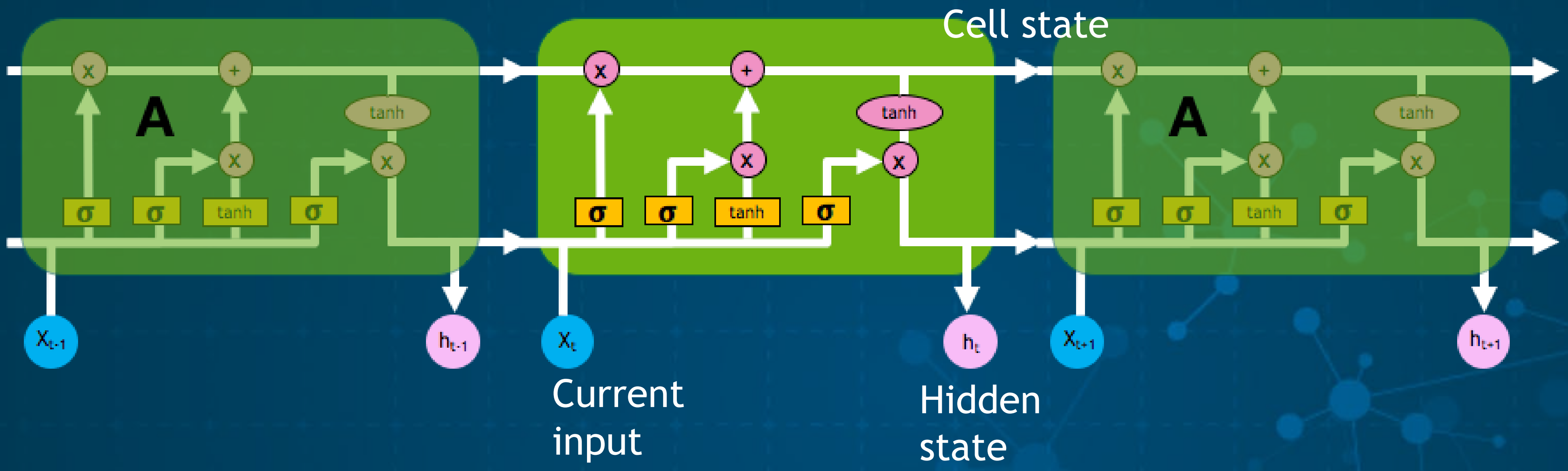
Time-series
Multivariate Adaptive Regression Splines



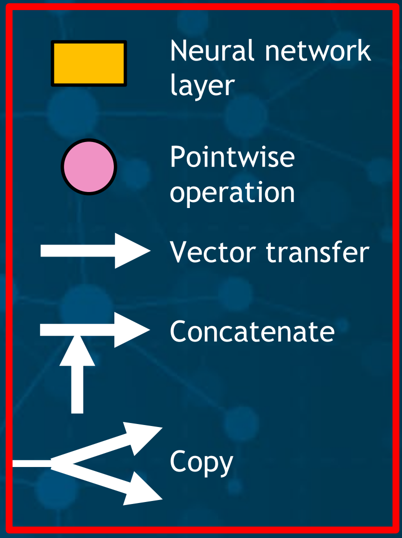
1. Useful for identifying nonlinear structure in time series
2. Non-parametric
3. Autoregressive: divide time-series into optimal subdomains to fit splines
4. Predicting microstructure evolution trajectories in PC space
5. Use m most recent time steps to predict N+1, N+2,…

Long Short-Term Memory Network

1. LSTM is a special kind of a recurrent neural net (RNN):
   Network with loops in them allowing information to persist (i.e., memory)
2. Looping connect previous information to current: TIME HISTORY!
3. Uses previous states, and current input
4. Learn/forget gate (internal structure) used to form long-term memory (known as cell state)and short-term memory (hidden state)
5. Predicting microstructure evolution trajectories in PC space
6. Use entire history to predict N+1, N+2,…

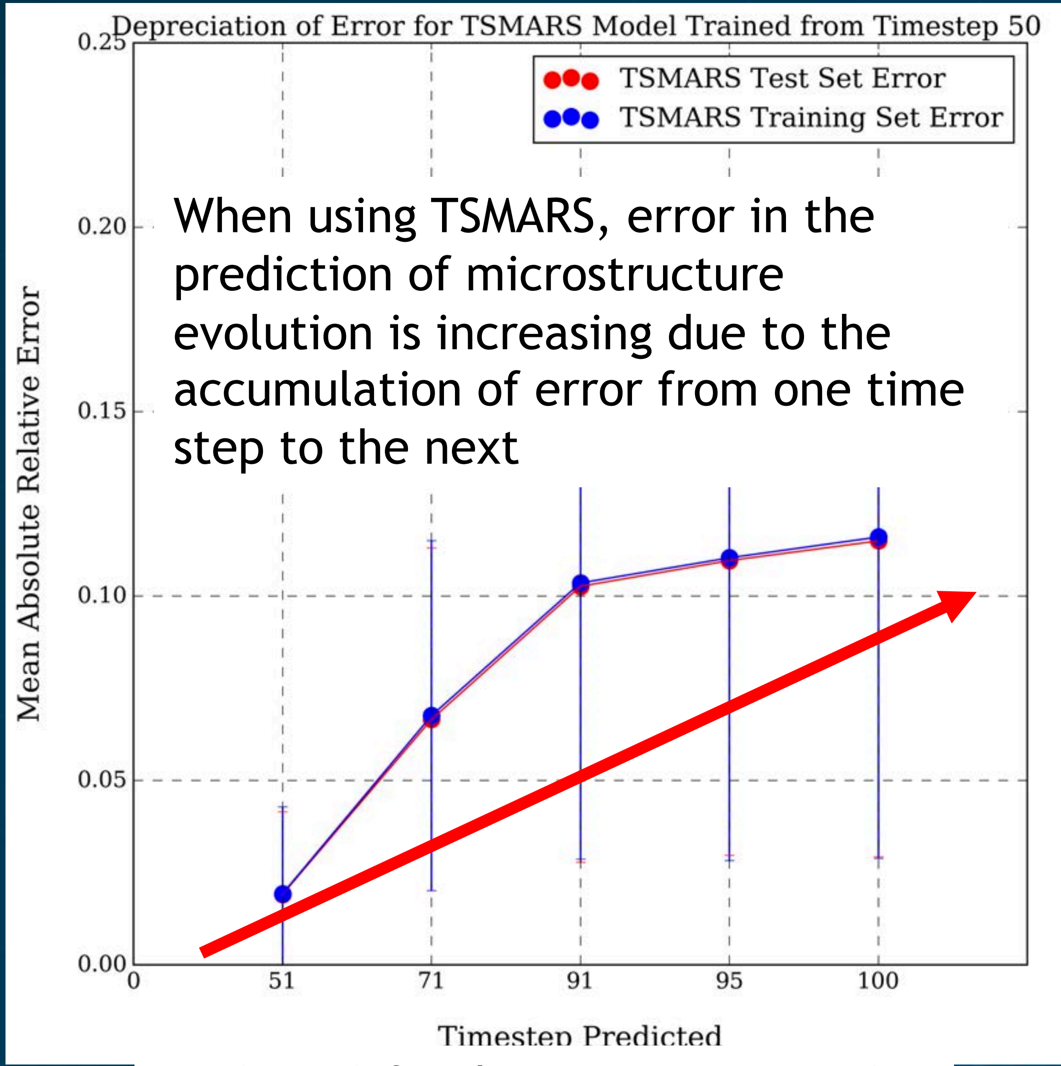


Nomenclature



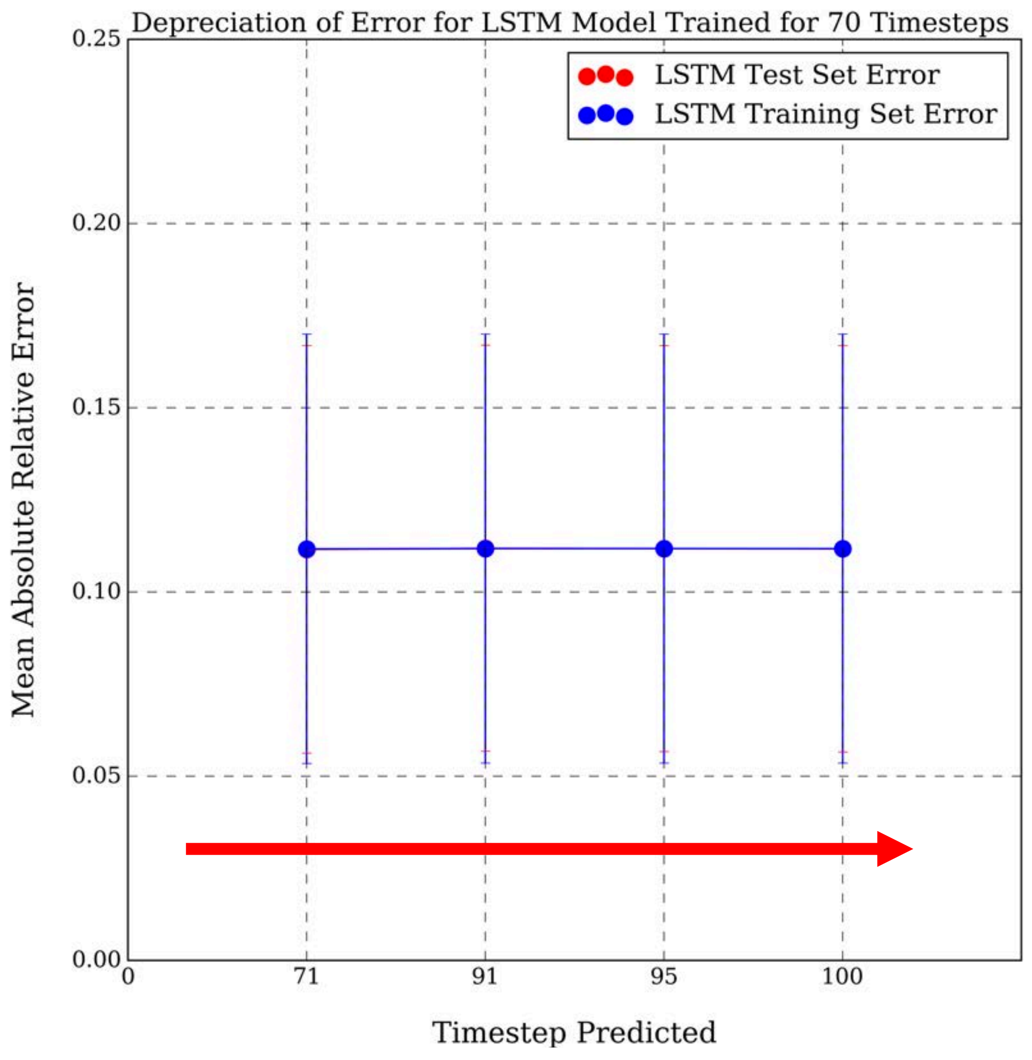
Why Do We Need A Deep Learning Strategy?

TSMARS



TSMARS for data augmentation?

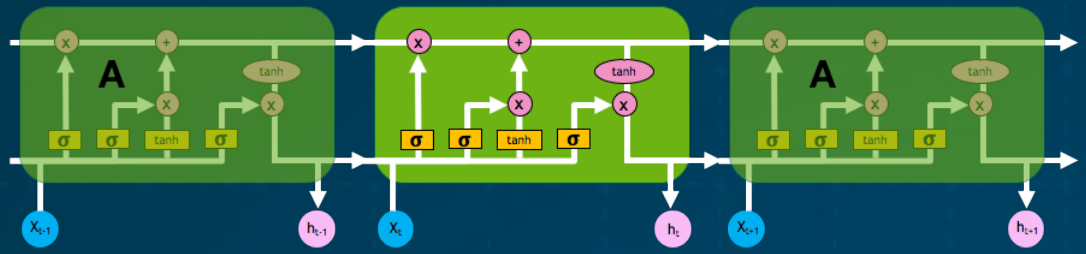
LSTM



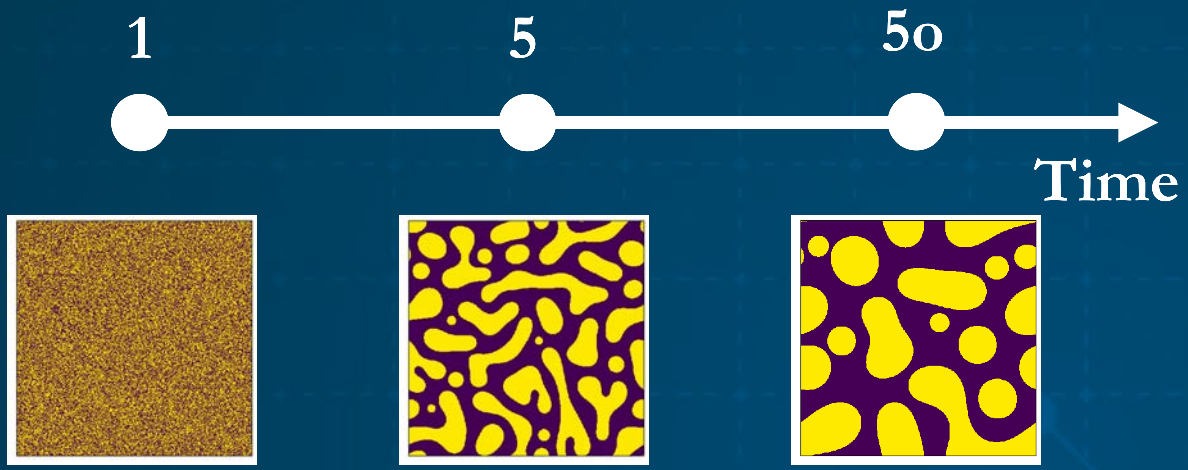
LSTM for PF acceleration?

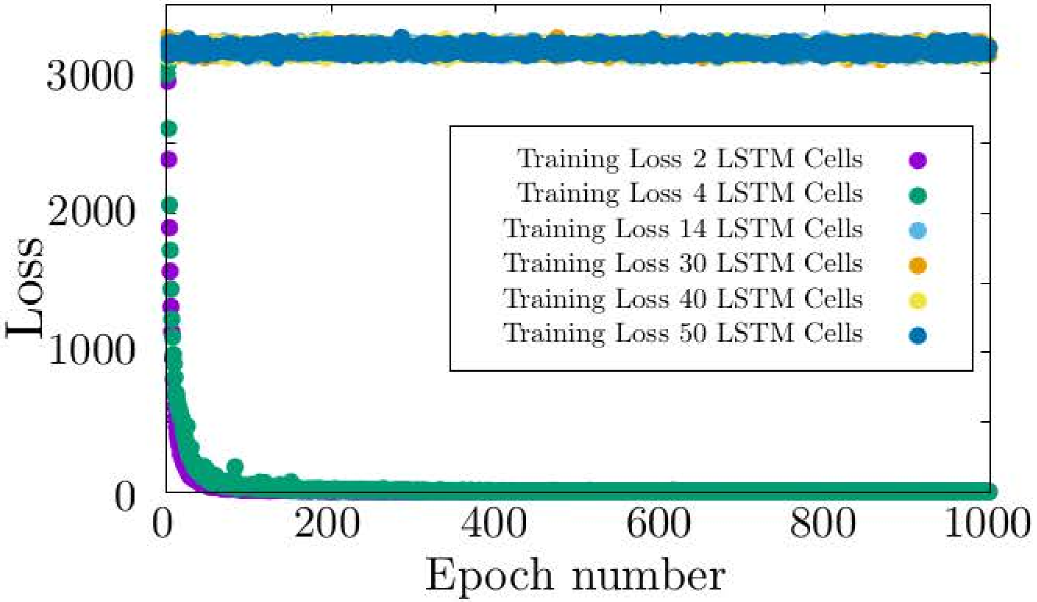
OPTIMUM LSTM ARCHITECTURE

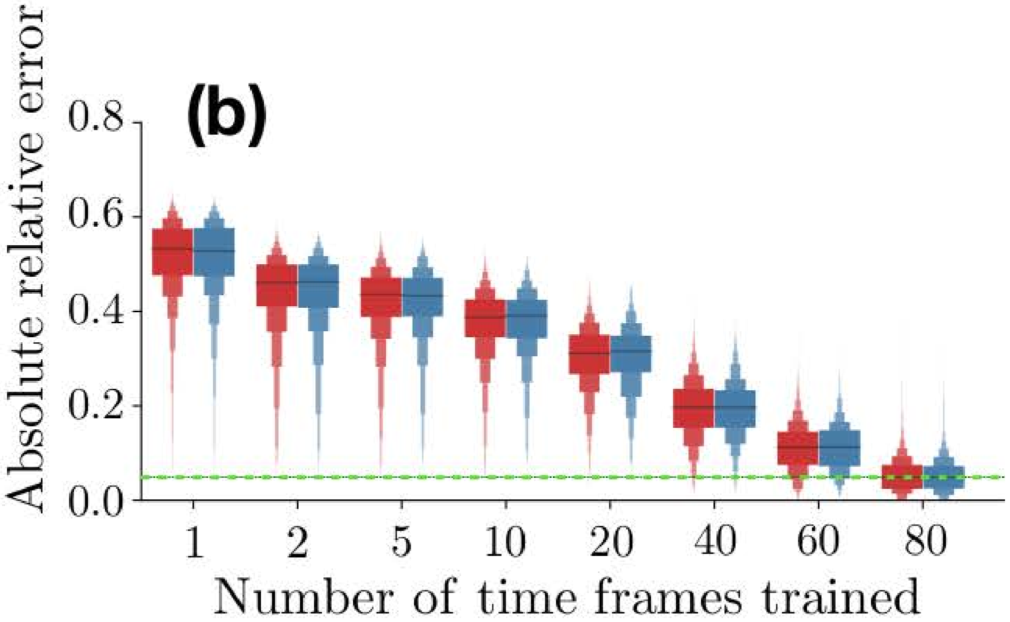
Number of LSTM cells:



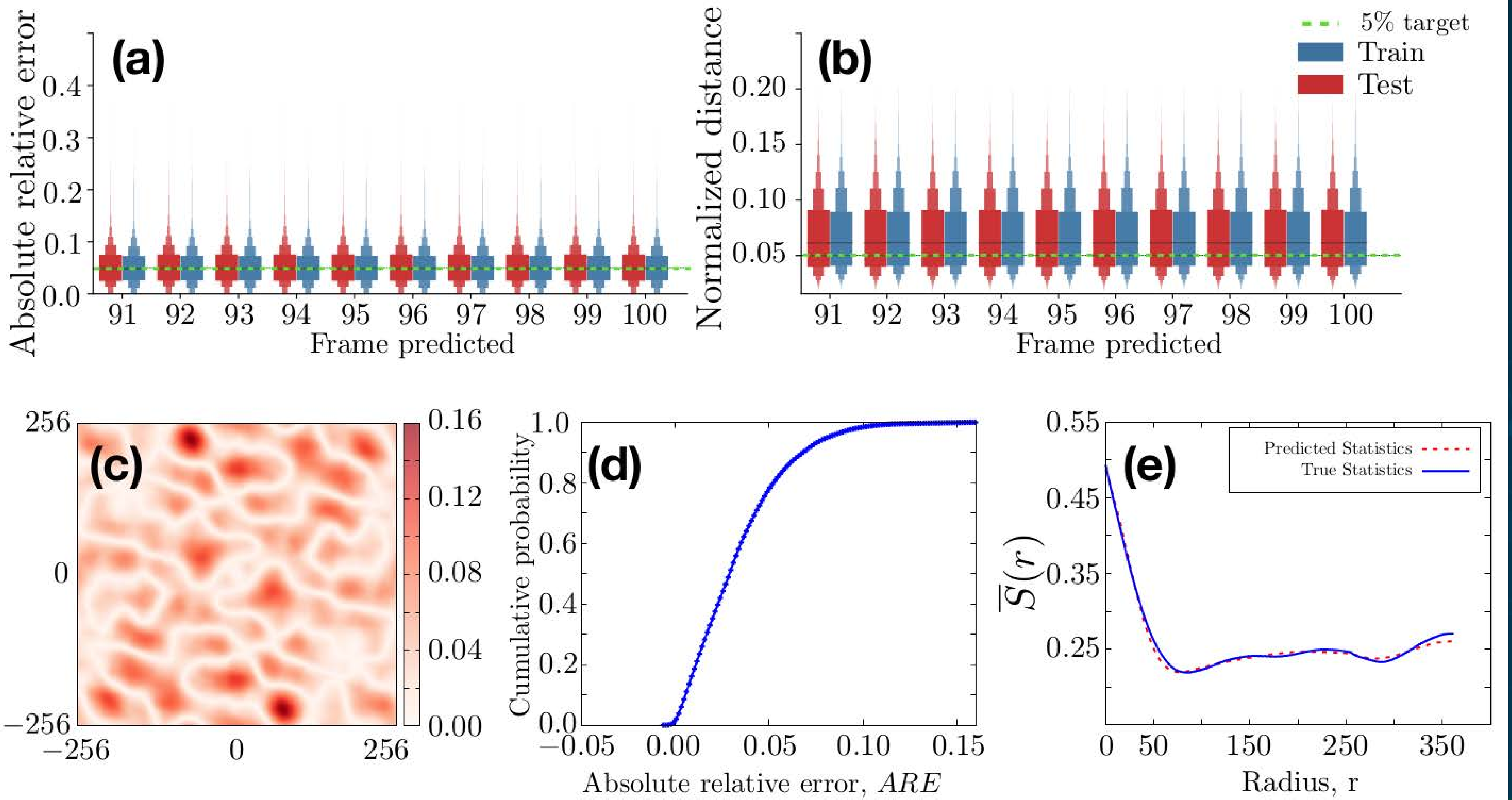
Number of time frames needed for training:







Performance of LSTM-Trained Model



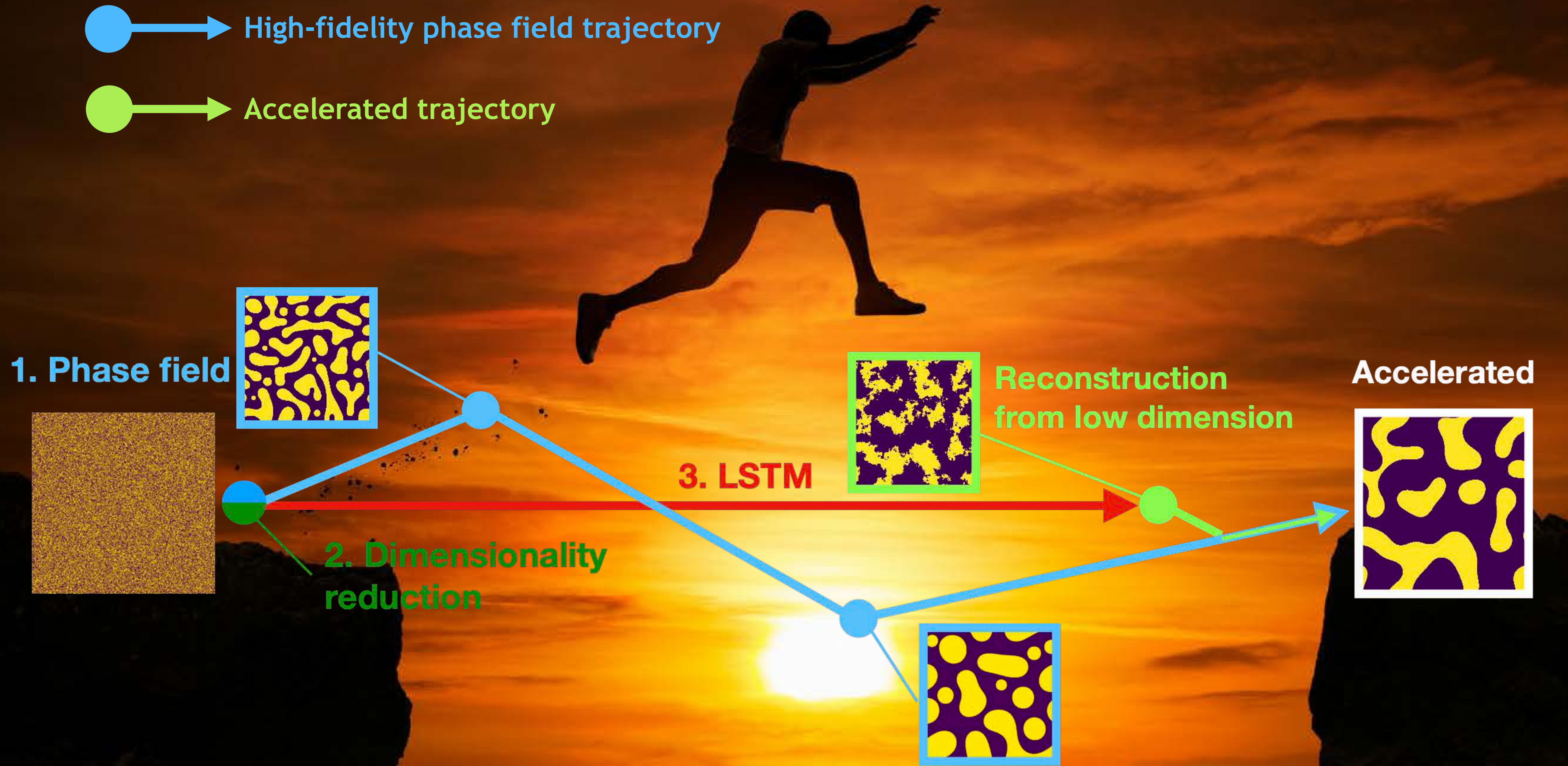
Computational Efficiency

	High-fidelity	LSTM-trained
1 simulation for 5M time steps	96 mins	0.06s
50,000 simulations	~9 year and 1 month	50 mins

Our LSTM-trained framework is more than 42,000 faster than the high-fidelity simulation with comparable accuracy!

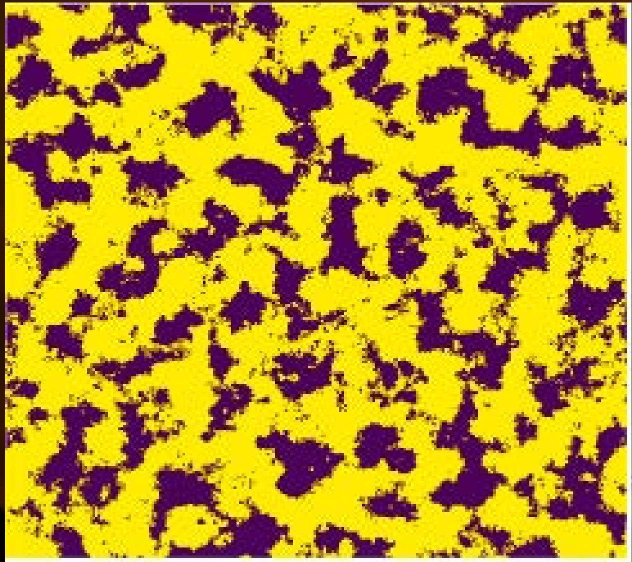
Opens a promising path forward for discovering, understanding and predicting evolutionary microstructural phenomena

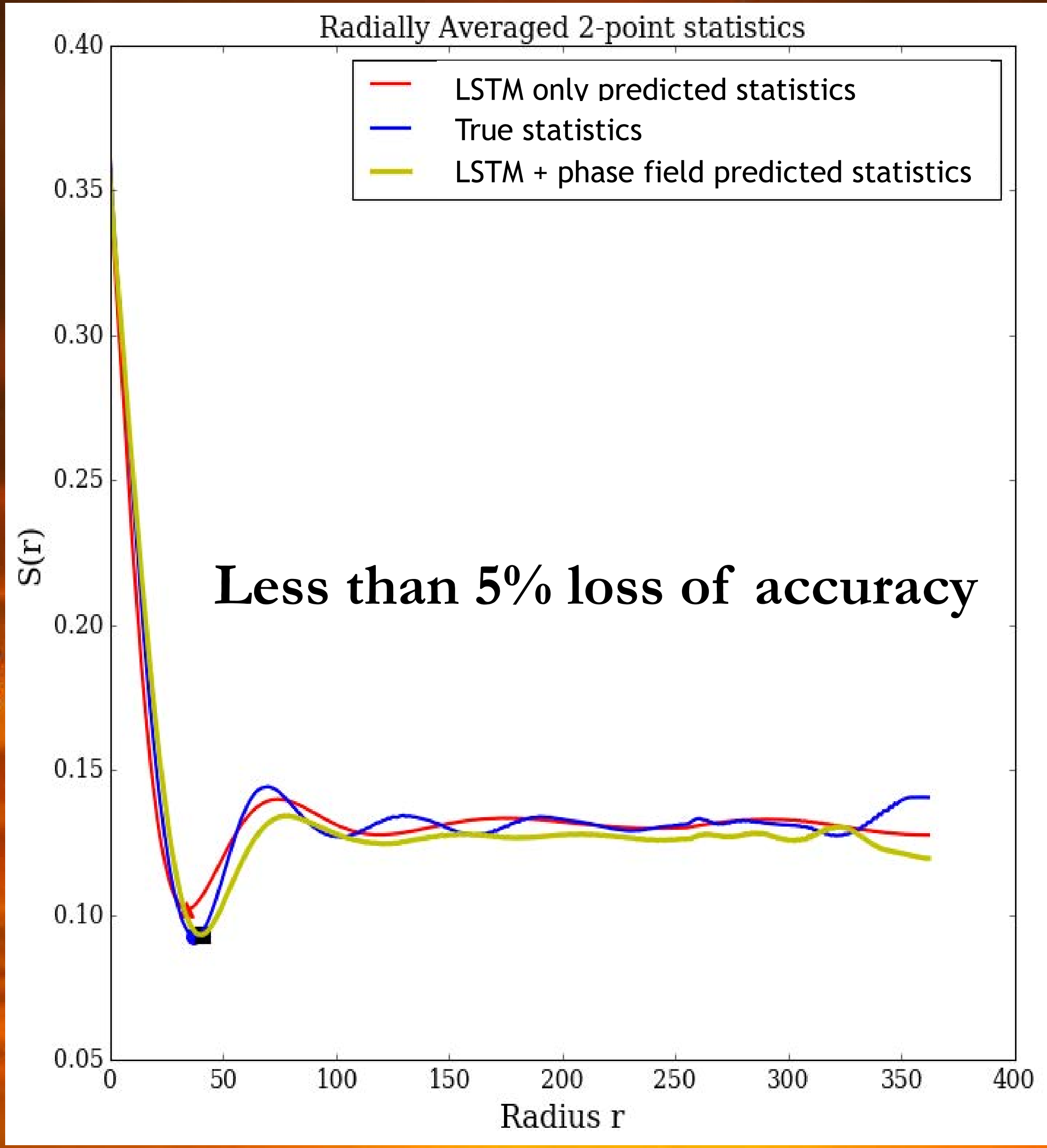
Accelerating Microstructure Evolution predictions: Step 4: Leaping in Time Using Machine-learned Surrogate



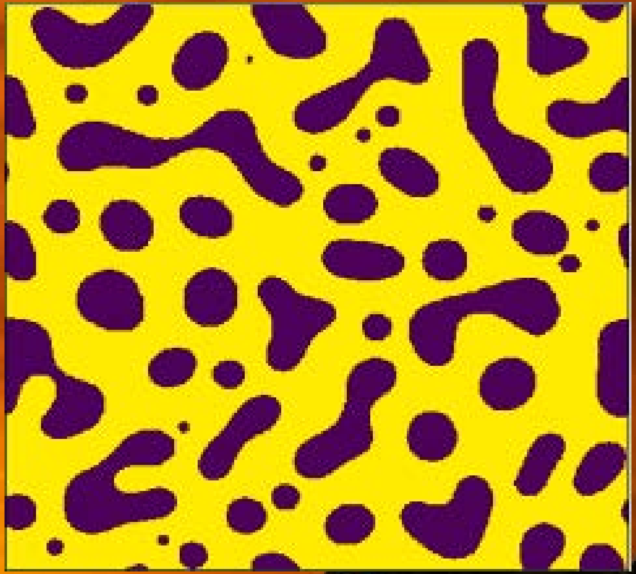
Accelerating Microstructure Evolution predictions: Leaping in Time Using Machine-learned Model

LSTM only



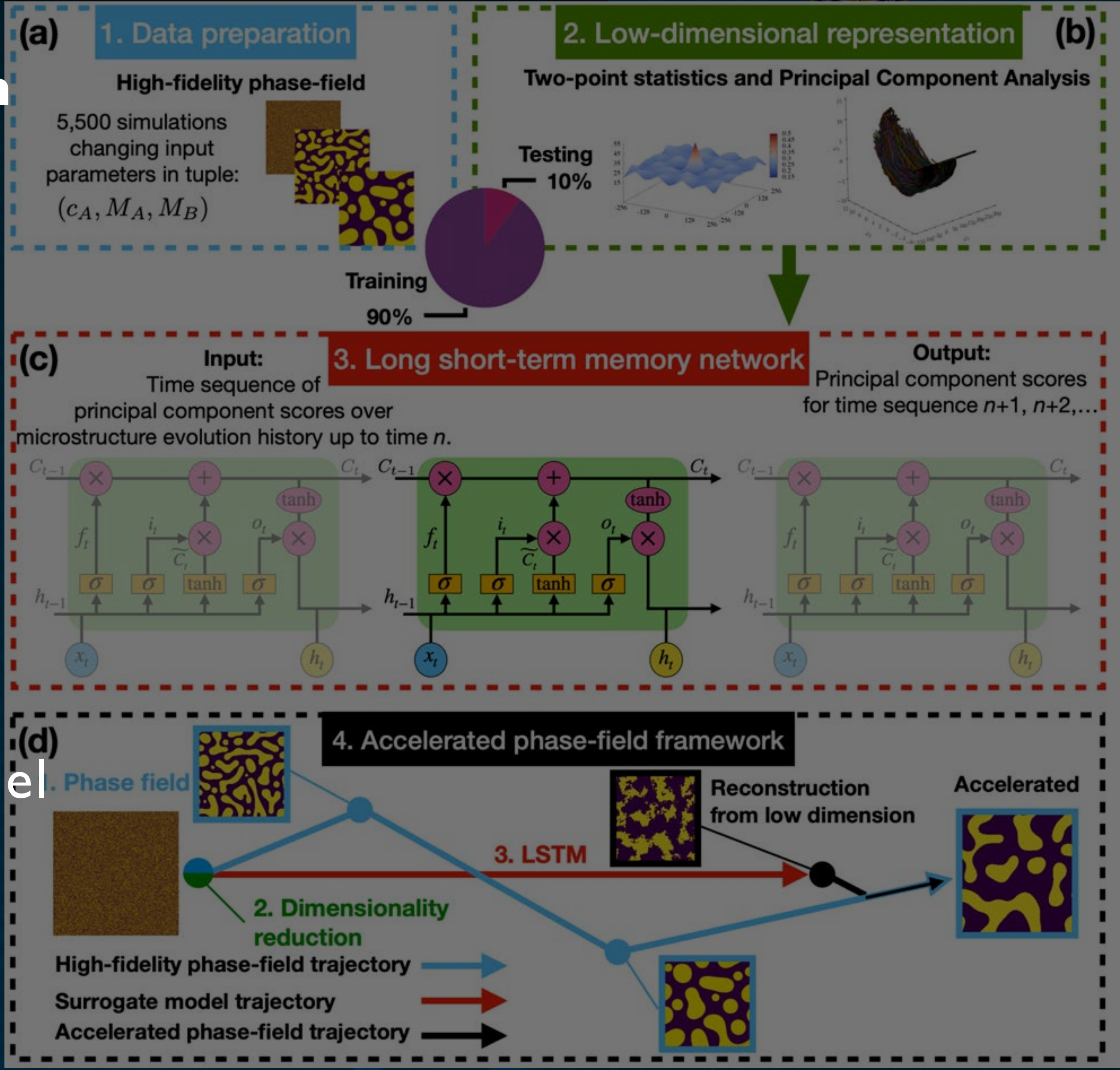


LSTM + phase-field



Moving Forward

- Reframing microstructure evolution as a multivariate time-series problem
  - Using LSTM to learn long-term patterns in reduced space
- Performance comparable to high-fidelity PF capabilities
  - >42,000 faster
  - less than 5% loss in accuracy
- Automated workflow (with S. Martin)
- Alternatives to PCA:
  - Autoencoders, GP latent variable model
- Alternatives to ML engine:
  - GRU, Independently RNN, plastic NN



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