SAND2020-8314PE

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

PRESENTED BY

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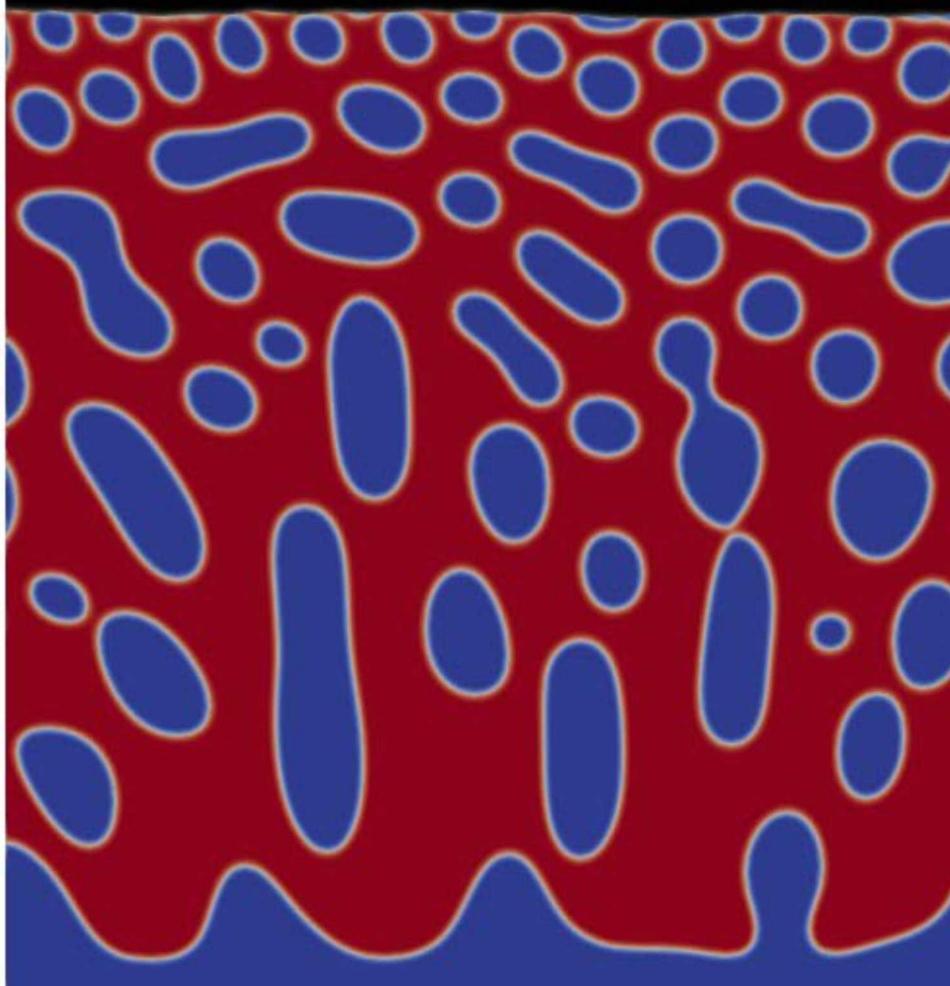

2020 MLDL Workshop

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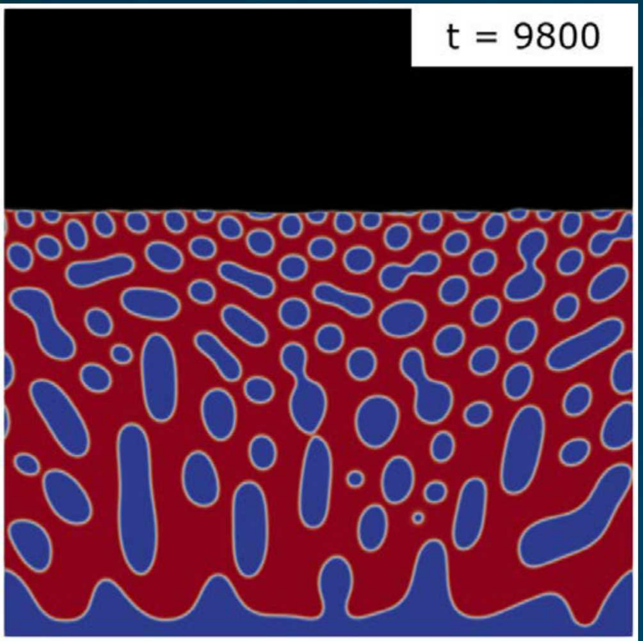
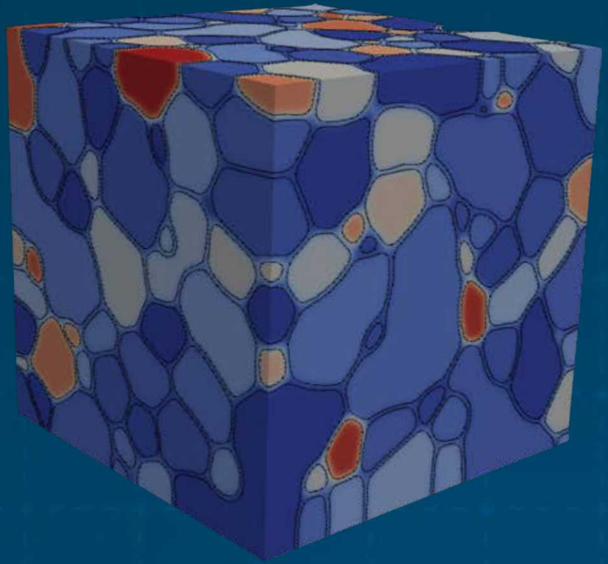
Predicting the Evolution of Microstuctures

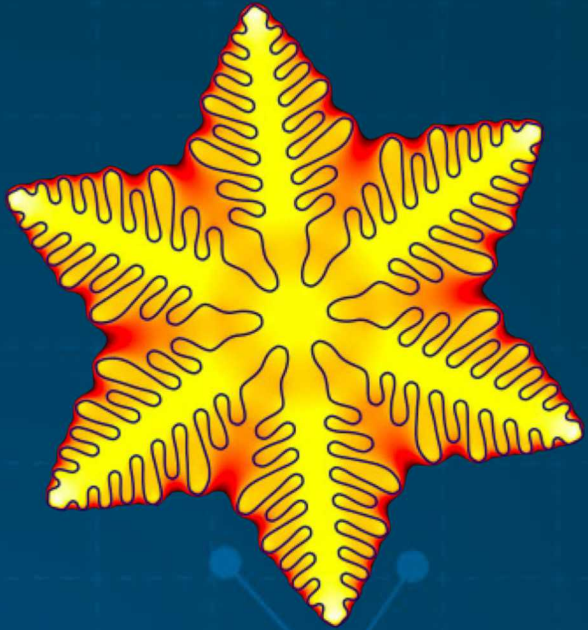
Thin-film deposition



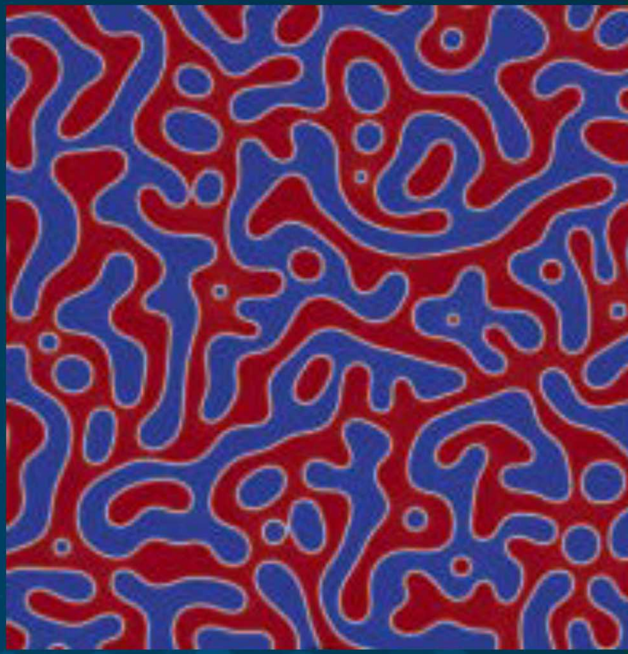
Grain growth



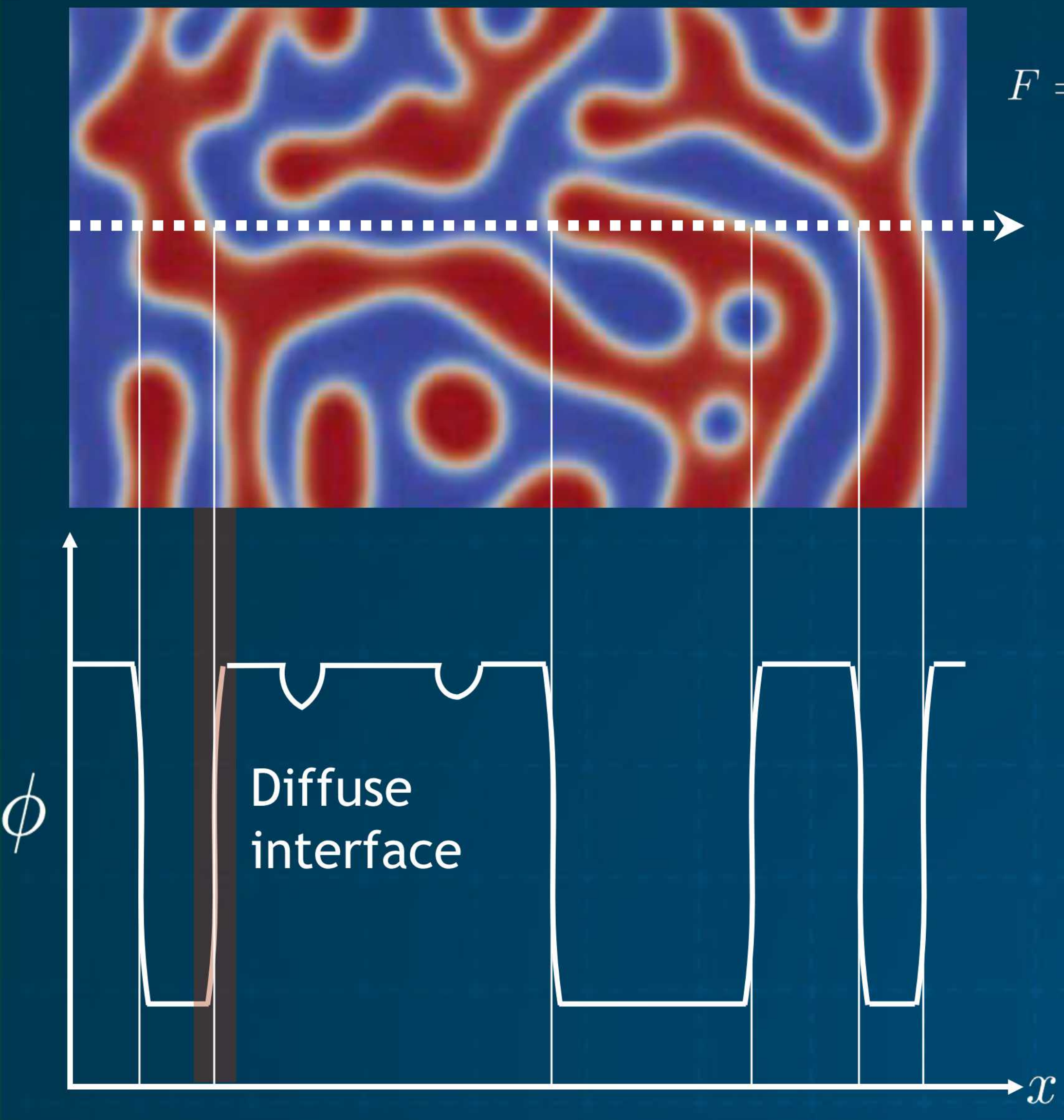
Solidification



Phase separation



Phase Field 101



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

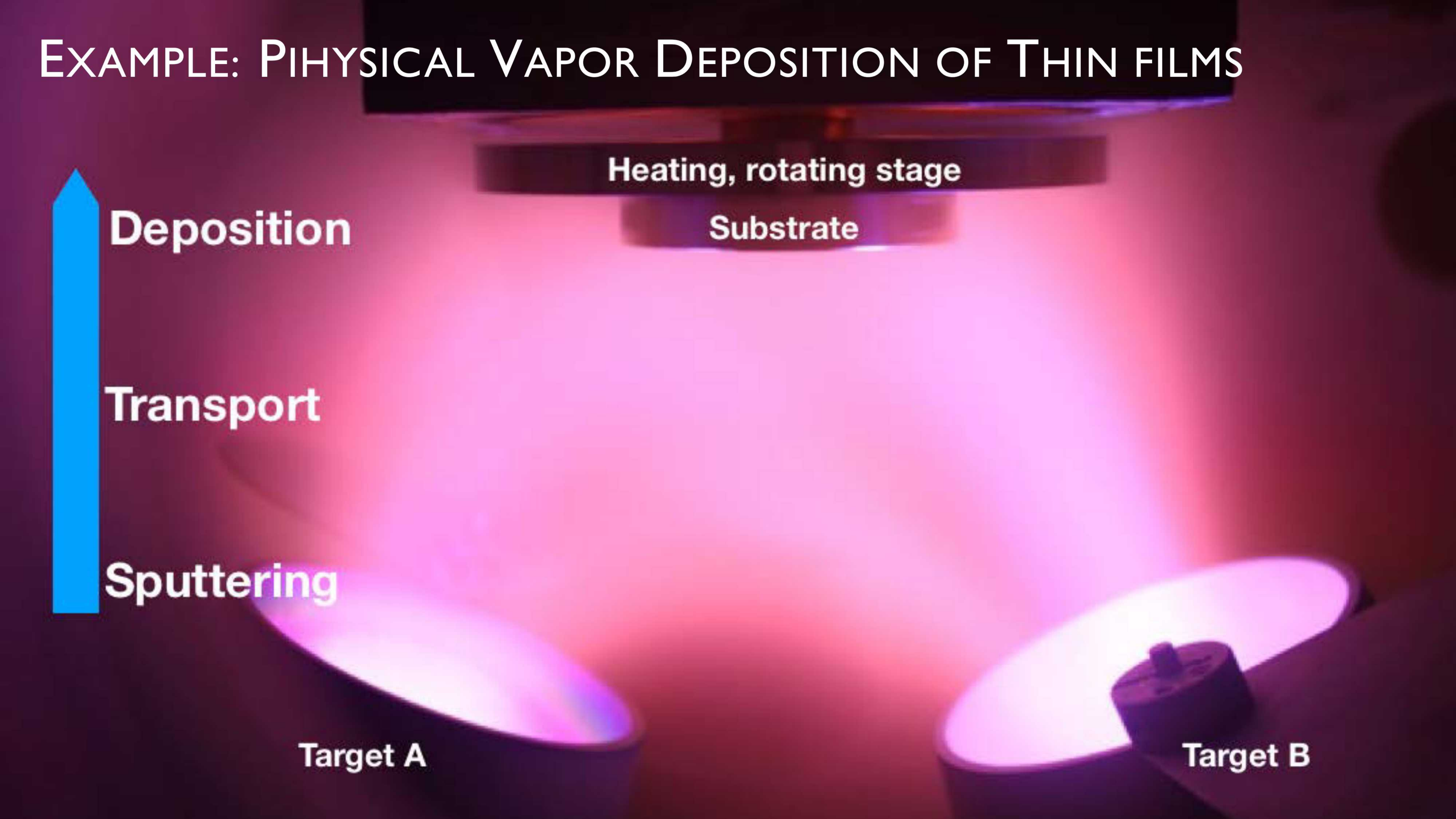
Allen-Cahn: Non-conserved

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

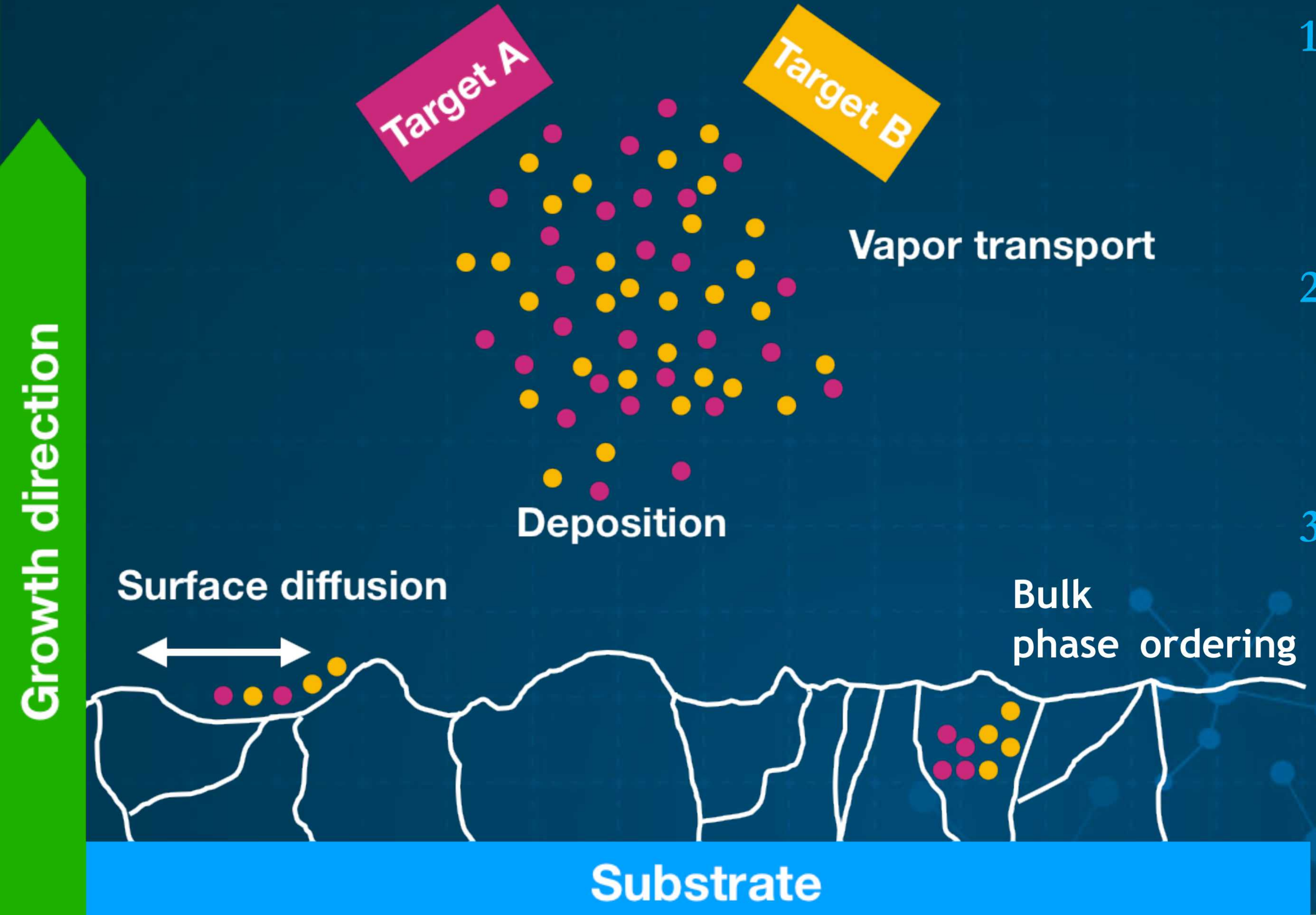
Cahn-Hillard: Conserved

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

Example: Pihysical Vapor Deposition of Thin films



Modeling PVD Using Phase-Field



1. **Explicitly model vapor transport**
   …so we can model multiple PVD processes
2. **No artificial deposition of vapor**
   …so we can capture hillock formation
3. **Account for surface and bulk diffusion into one model**
   …so we can account for the composition of surface vs. bulk phenomena

Modeling PVD Using Phase-Field

$$F = \int \left[\boxed{f_\phi + \frac{\kappa_\phi^2}{2} \left(\nabla \phi\right)^2} + s\left(\phi\right) \boxed{\left(f_{el} + f_c + \frac{\kappa_c^2}{2} \left(\nabla c\right)^2 \right)} \right] d\Omega$$

Describing vapor/solid field

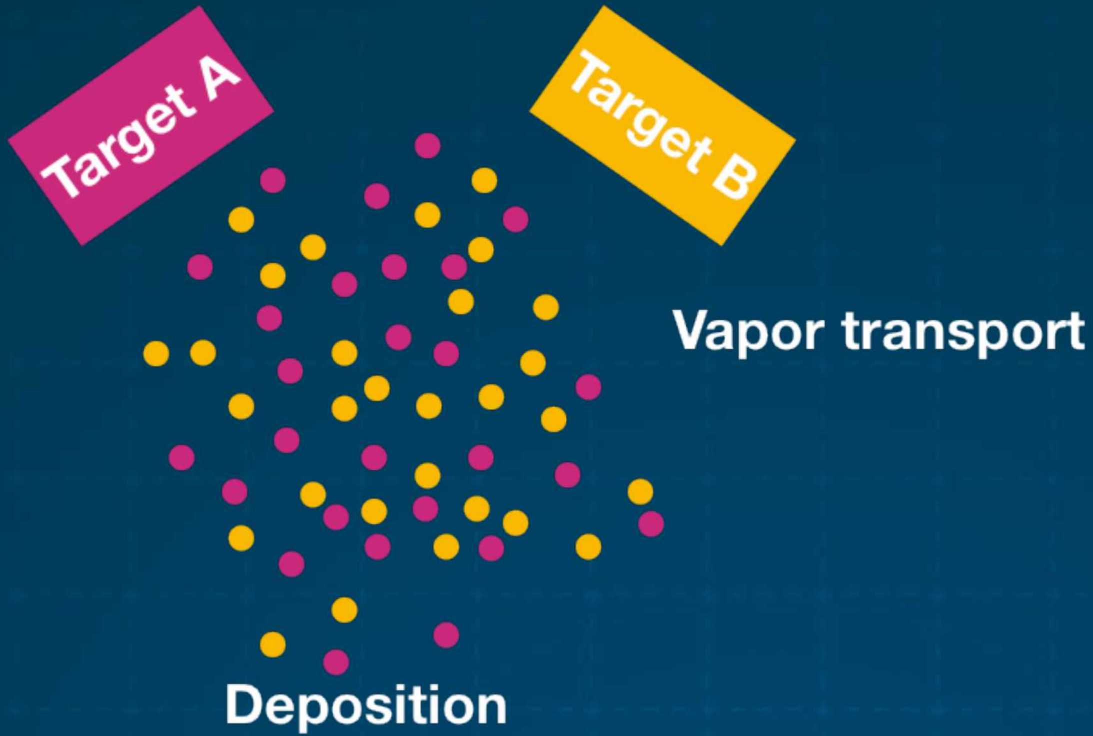
Only considered within the solid thin film

Describes concentration & elastic fields

Describes two-way coupling between elastic and concentration fields (Vegard)

Substrate

Transport & Evolution of Incident Vapor



$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D(\rho)\nabla \rho) - \nabla \cdot (\rho \vec{u}) - S\left(\vec{n}\right)$$

Convection-diffusion

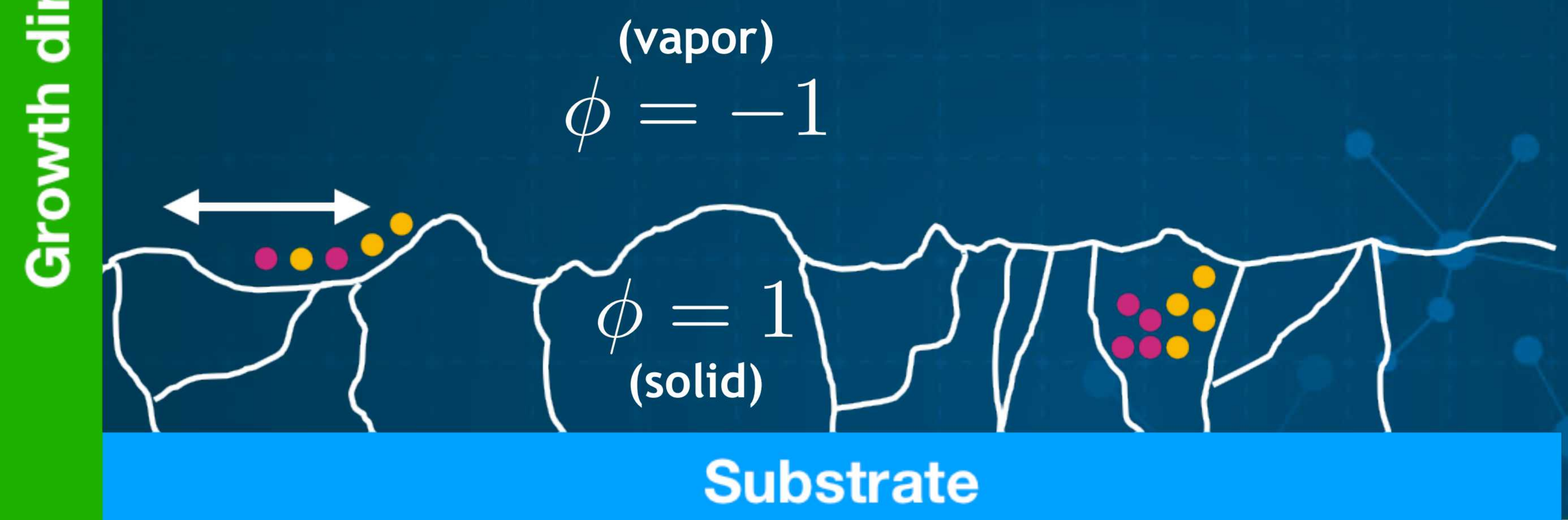
1. Local vapor pressure
2. Sputtering power (velocity)
3. Vapor density and velocity can be adapted to simulated various PVD processes
4. Random distribution of vapor phase initially
5. Source term to allow for removal of vapor that is being converted to solid at thin-film interface
6. Inclusion of LB capability in the future to include hydrodynamic effects (ALD, CVD)

Substrate

Kinetics of Thin-Film Growth

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \left(M(\phi) \nabla \frac{\delta F}{\delta \phi} \right) + S\left(\vec{n}\right)$$

1. Allows for arbitrary surface morphology formation
2. Captures surface-diffusion effects
3. Coupling of thin-film evolution to incident-vapor flux

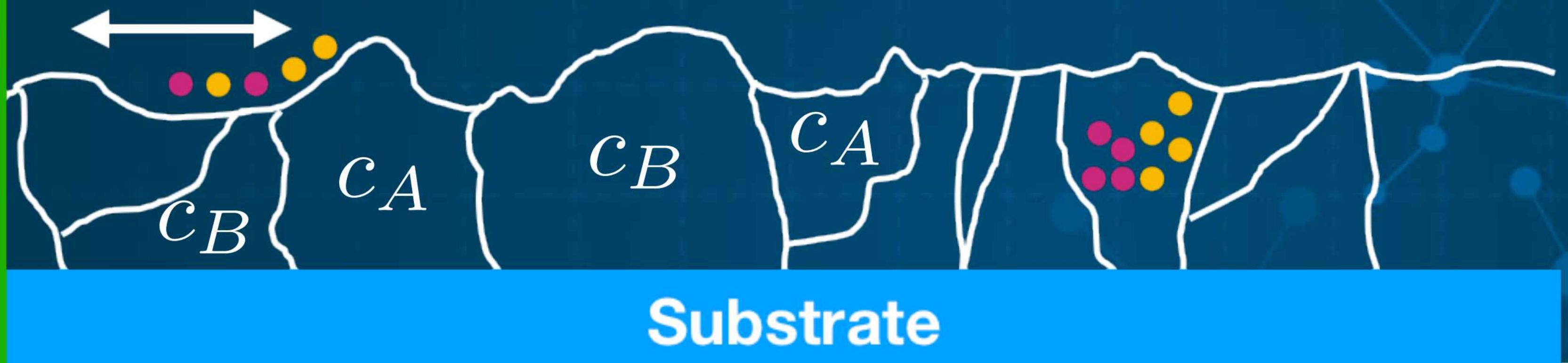


Phase Ordering in Thin-Film

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M(\phi, c) \nabla \frac{\delta F}{\delta c} \right)$$

$$M_c(\phi, c) = M^{\mathrm{Bulk}} + M^{\mathrm{Surf}}$$

1. Bulk or surface mobilities are selected through a **ϕ**-dependent switching function
2. Ensure that surface mobility is localized to vapor-solid interface
3. Explicitly capture both surface and bulk diffusion



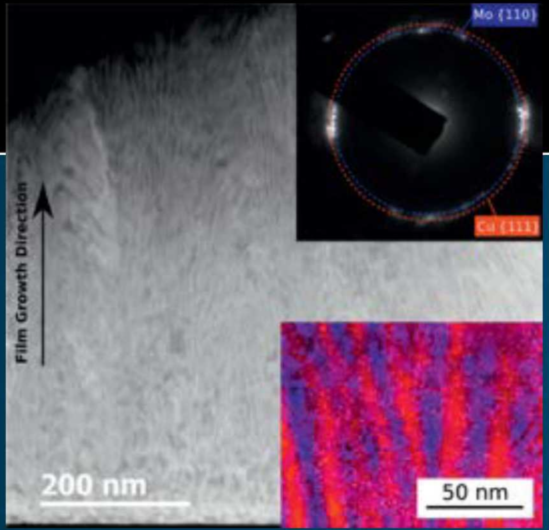
Modeling PVD Using Phase-Field

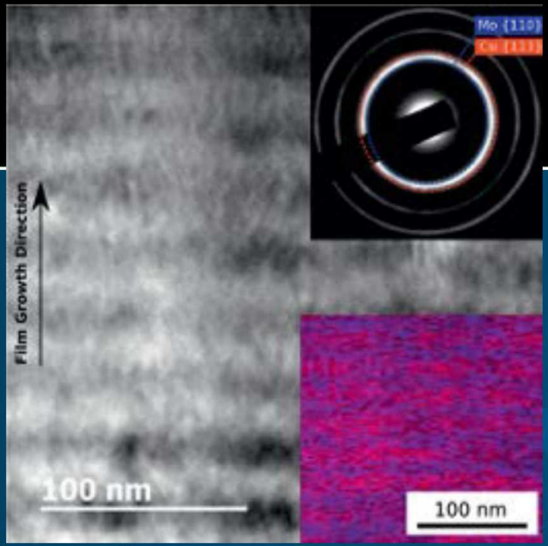
Target A Lateral Target B

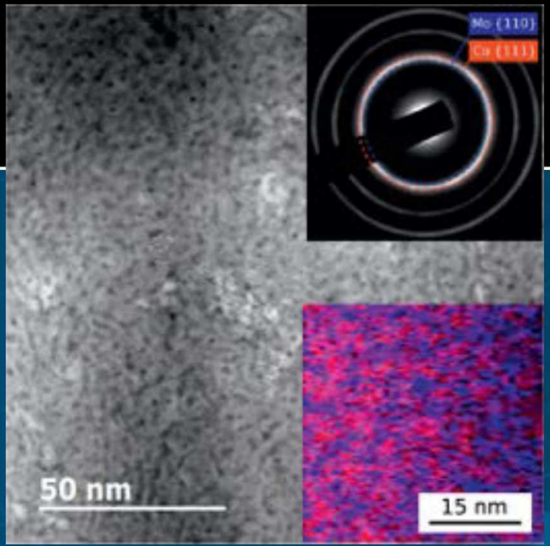
Target A Vertical Target B

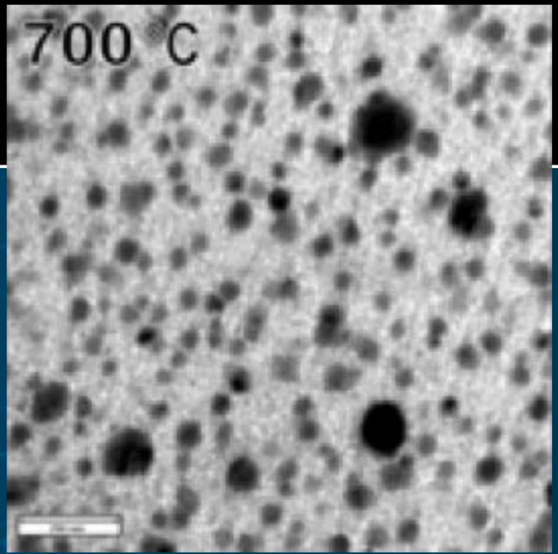
Target A Random Target B

Target A Nanoprecipitate Target B

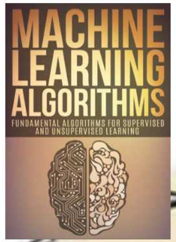


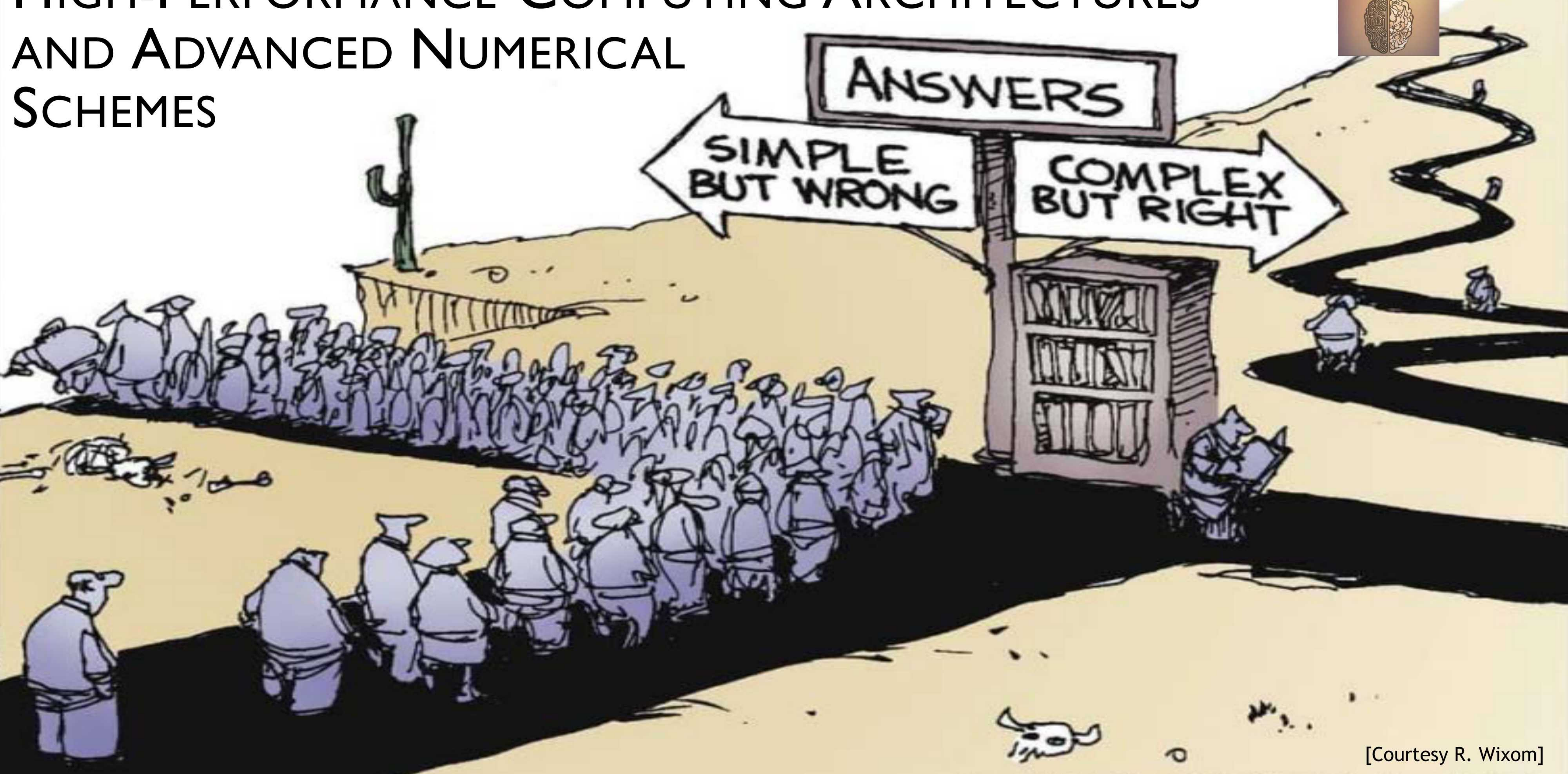






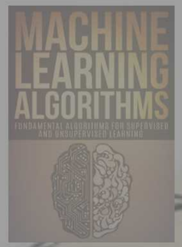
Current Efforts Focus on Leveraging High-Performance Computing Architectures and Advanced Numerical Schemes

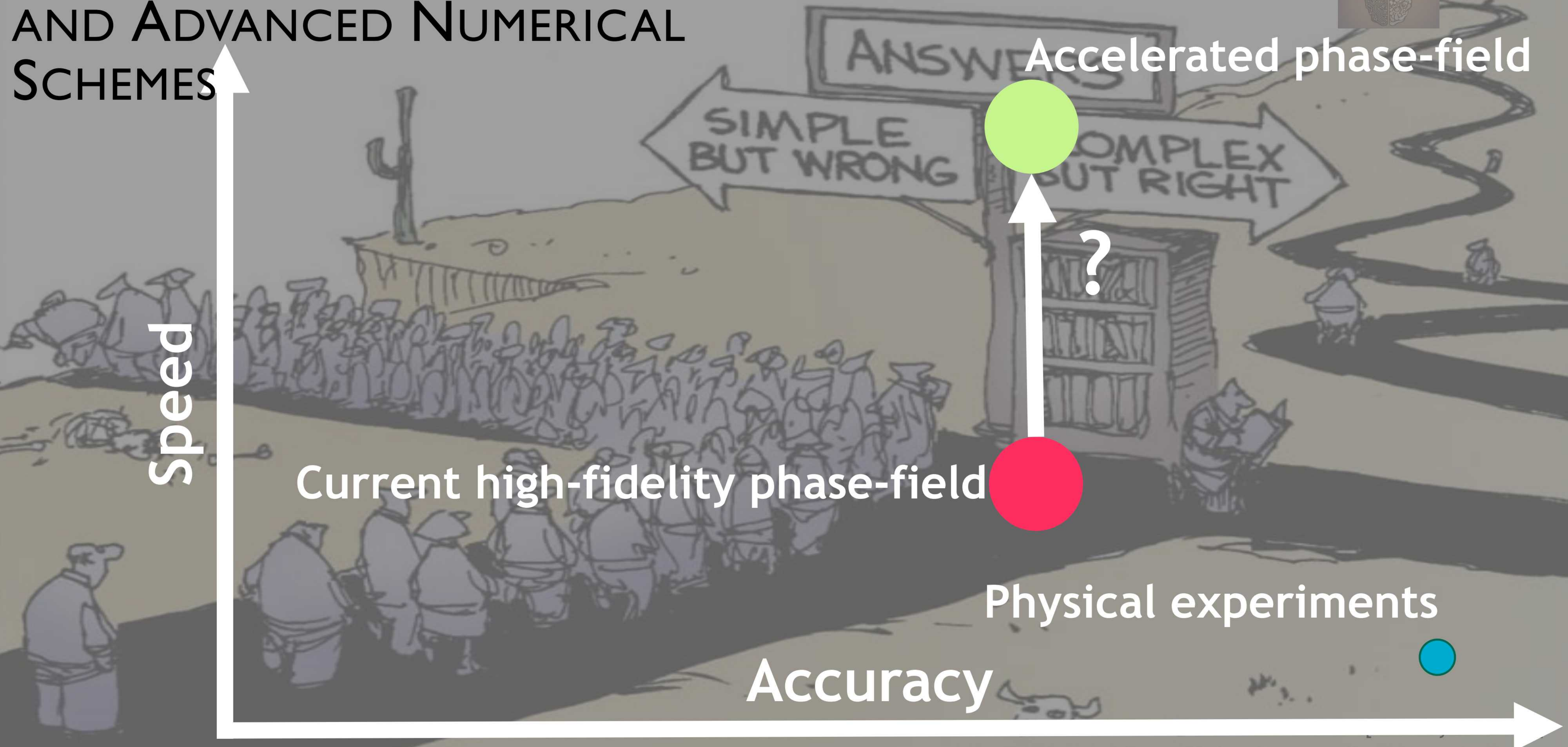




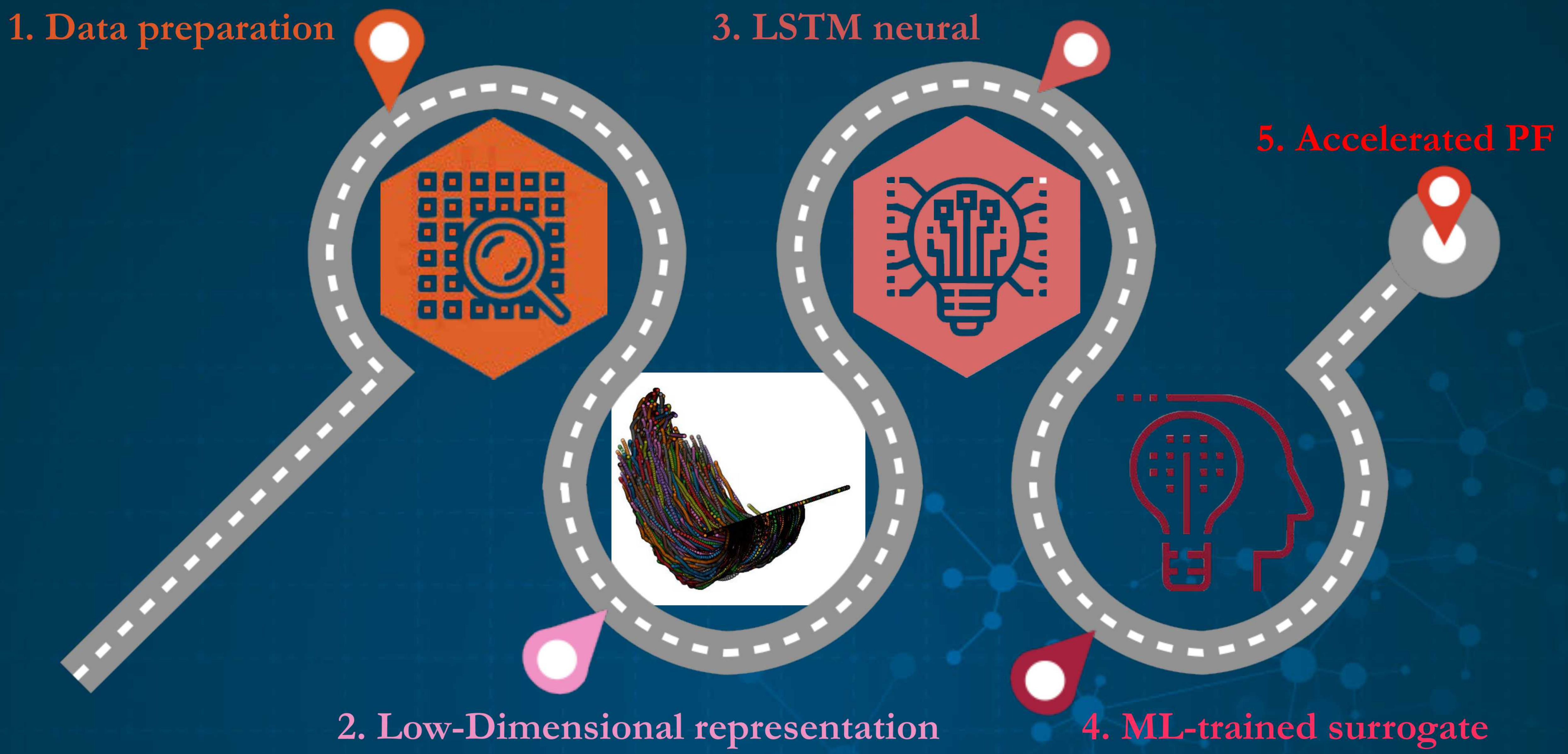
[Courtesy R. Wixom]

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

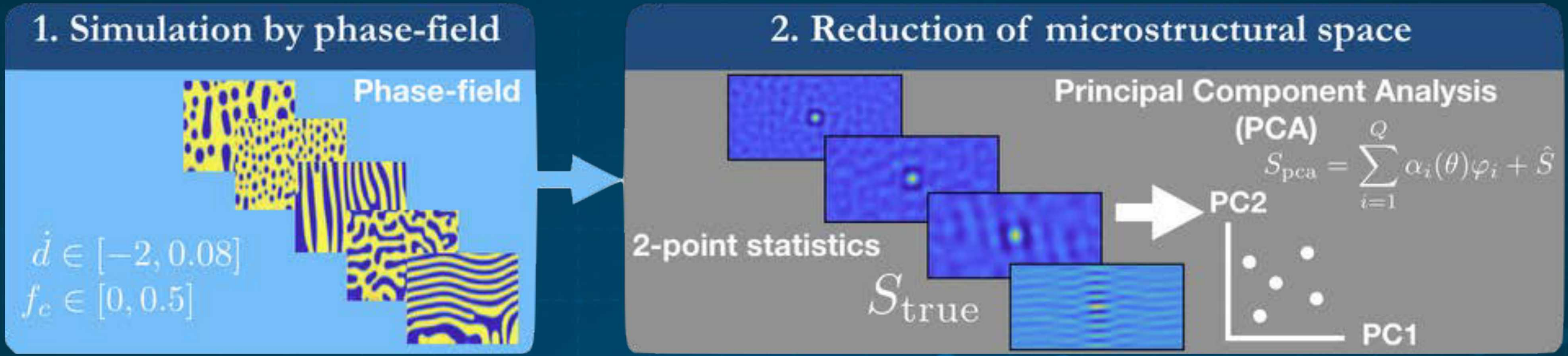




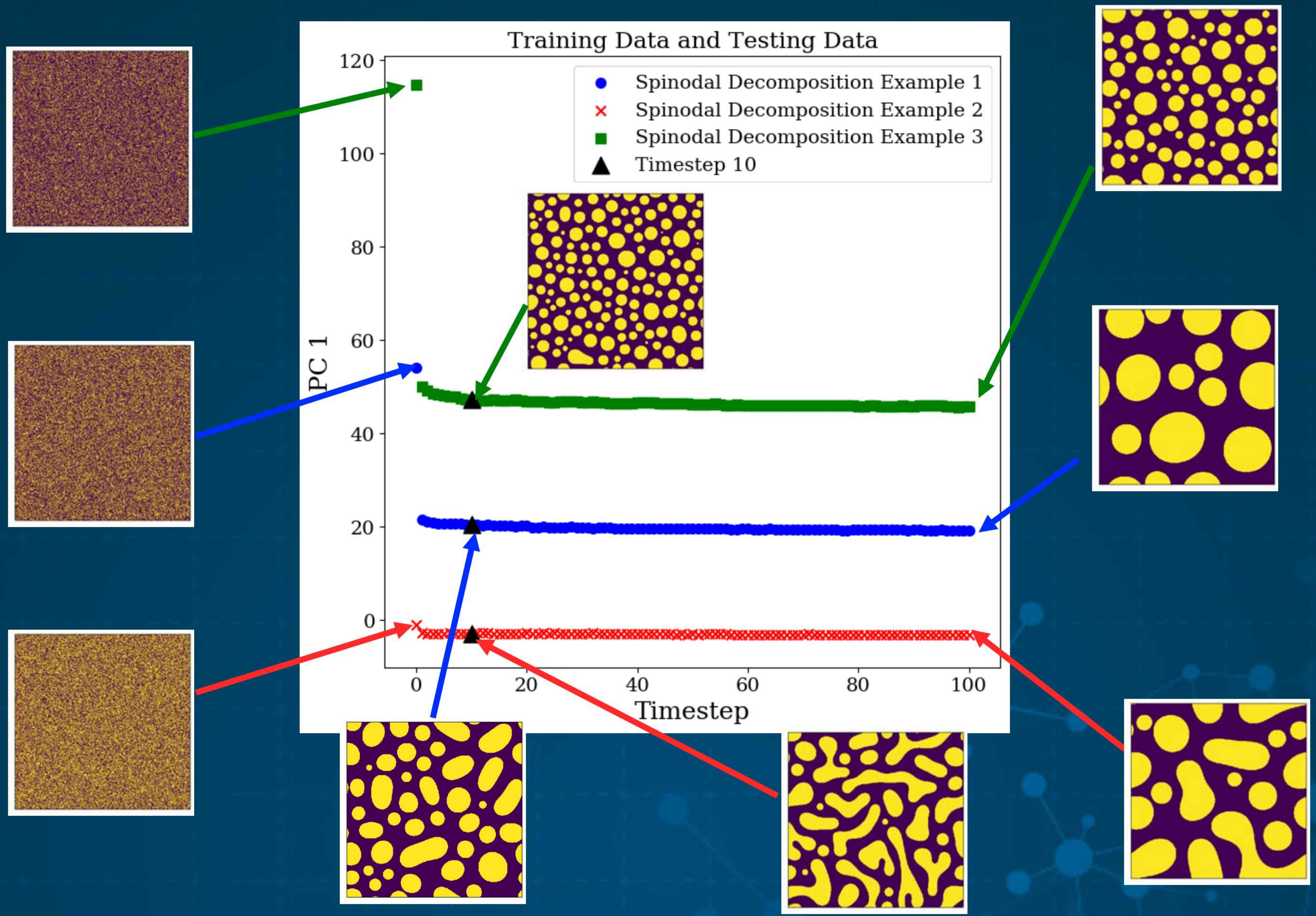
Algorithmic Approach



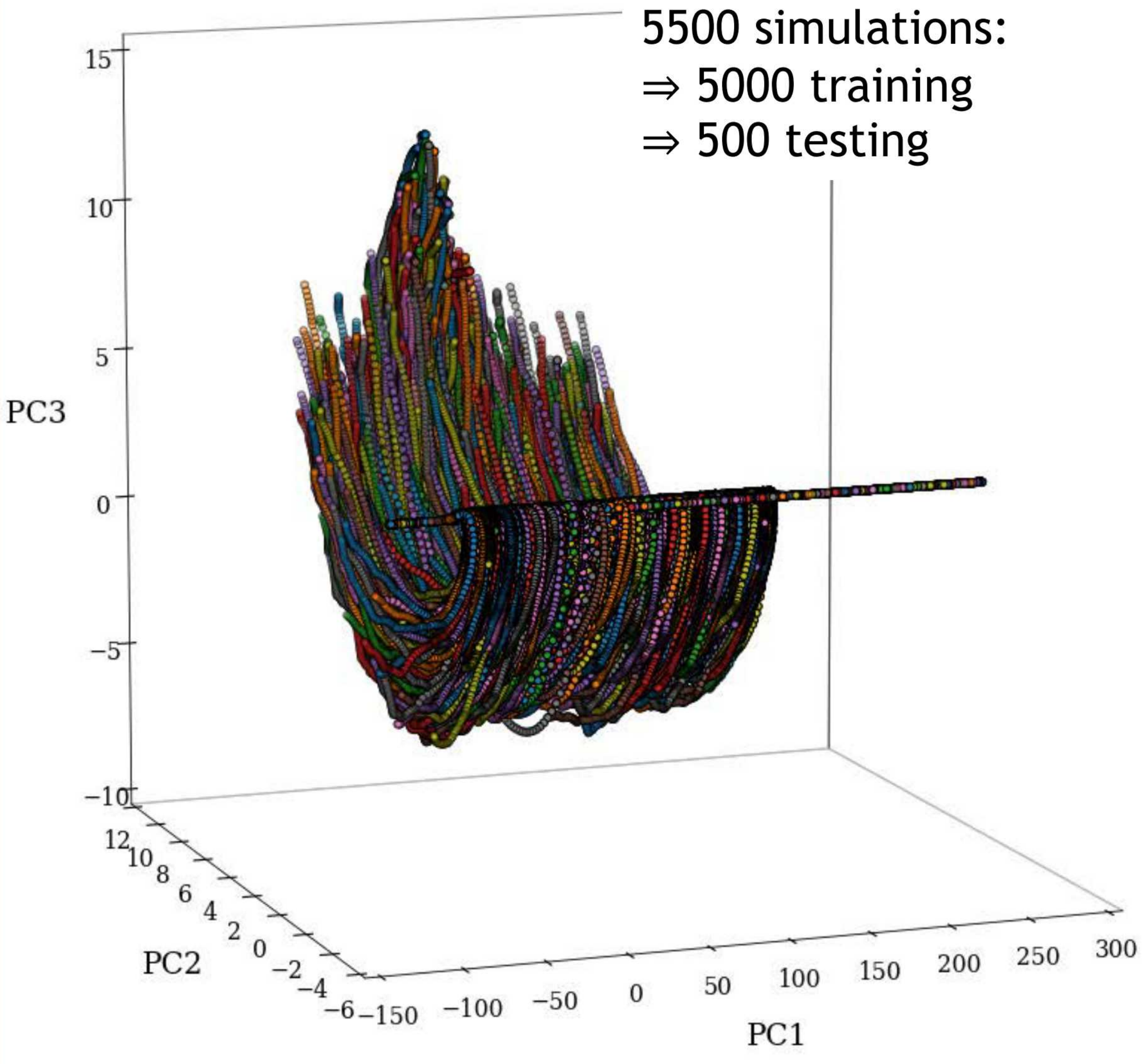
Dimensionality Reduction



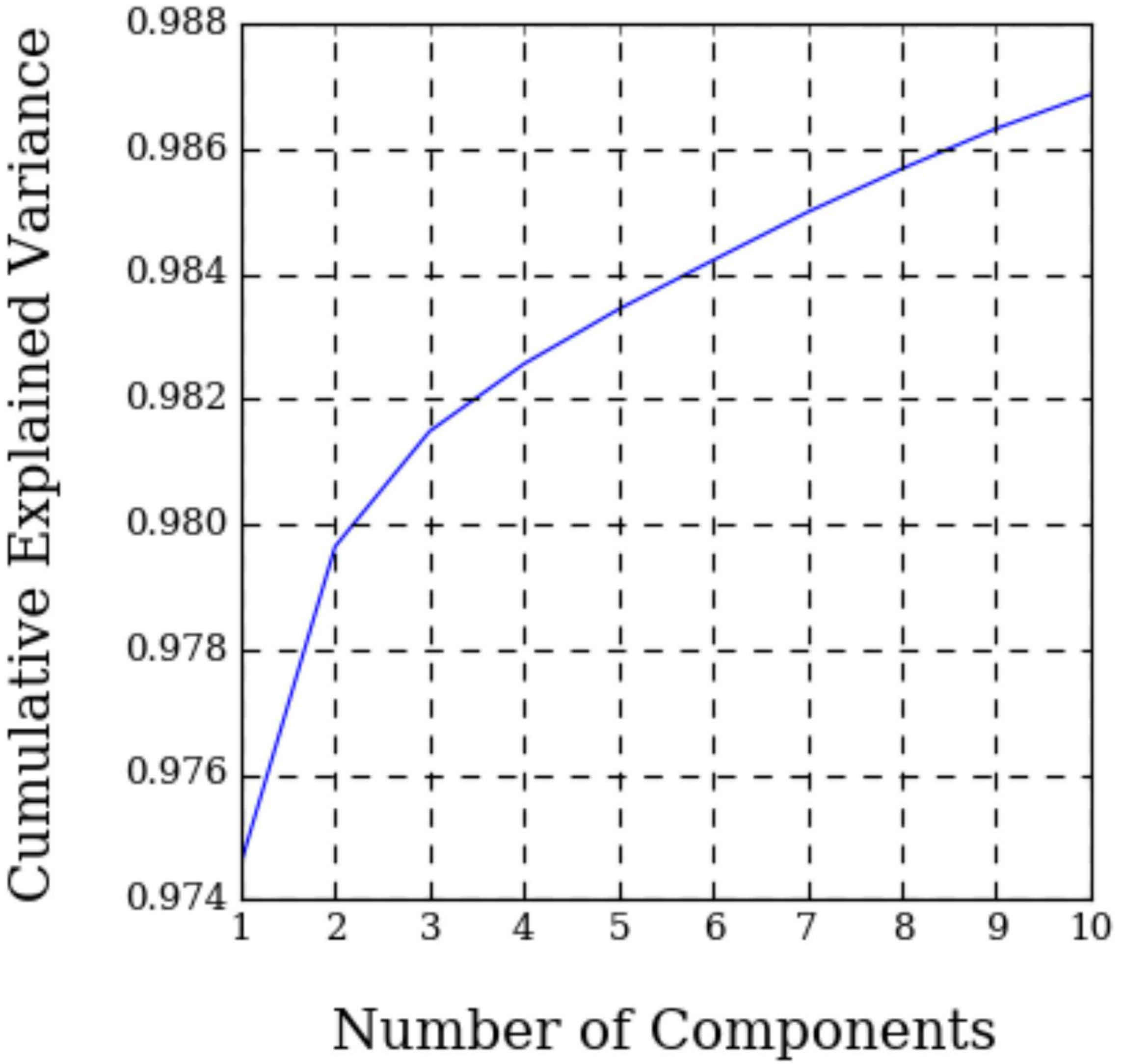
Microstructure Trajectory in PC Space



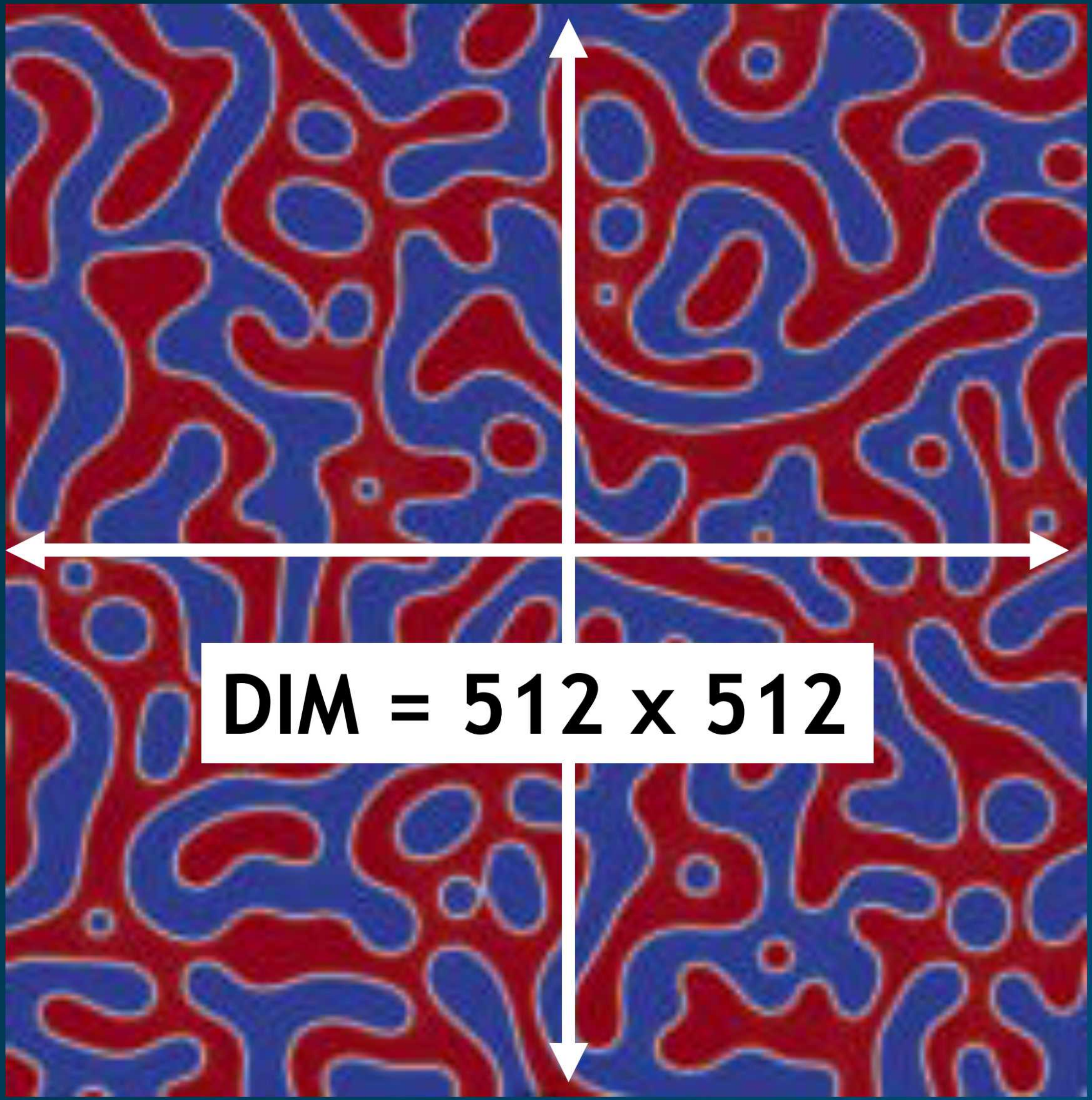
Microstructure Trajectory in PC Space

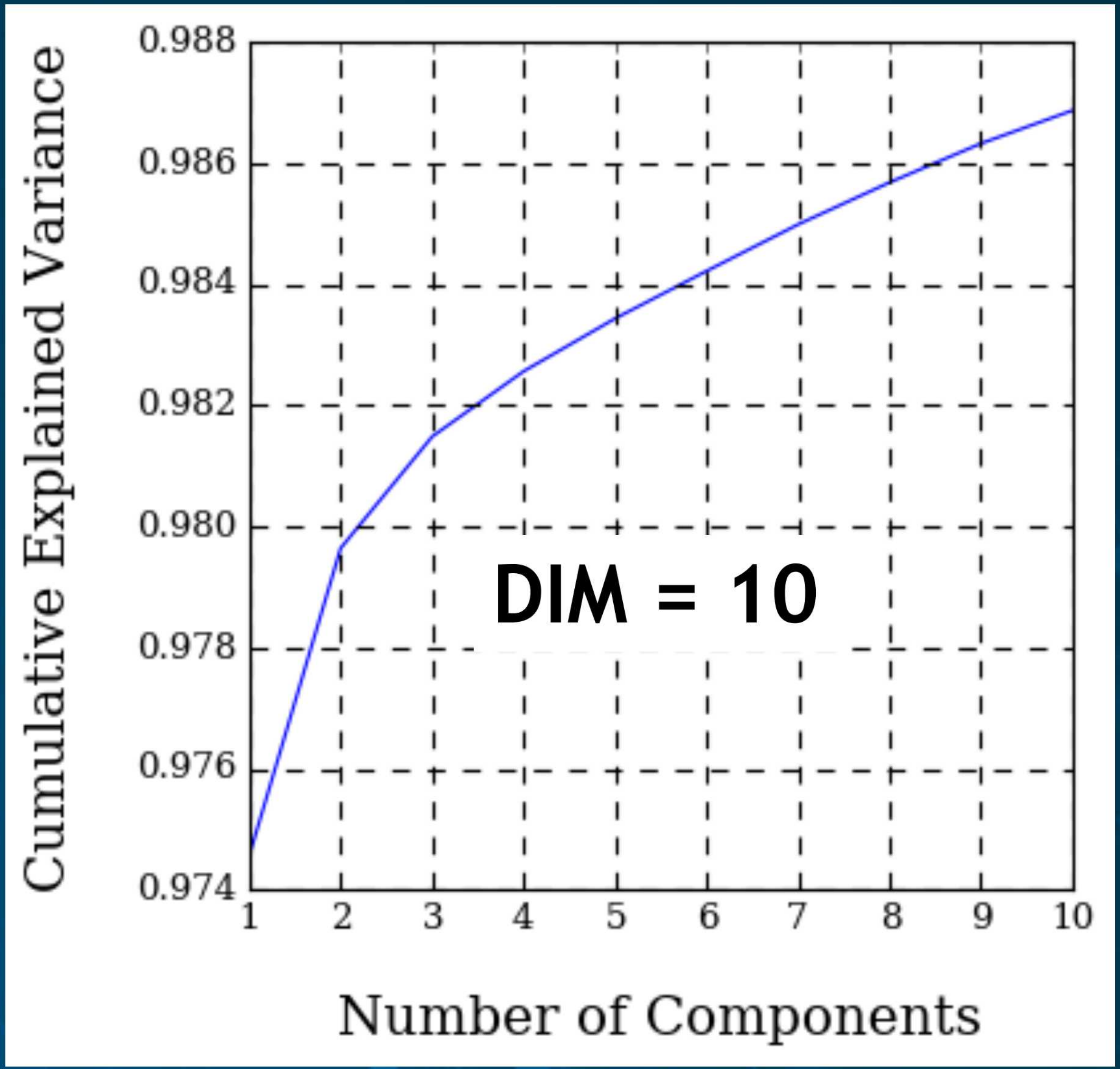


5500 simulations:
⇒ 5000 training
⇒ 500 testing



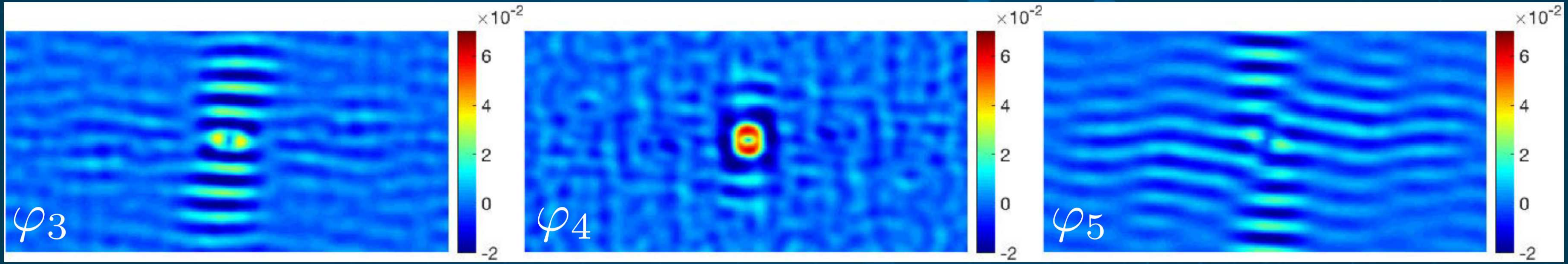
Dimensionality Reduction



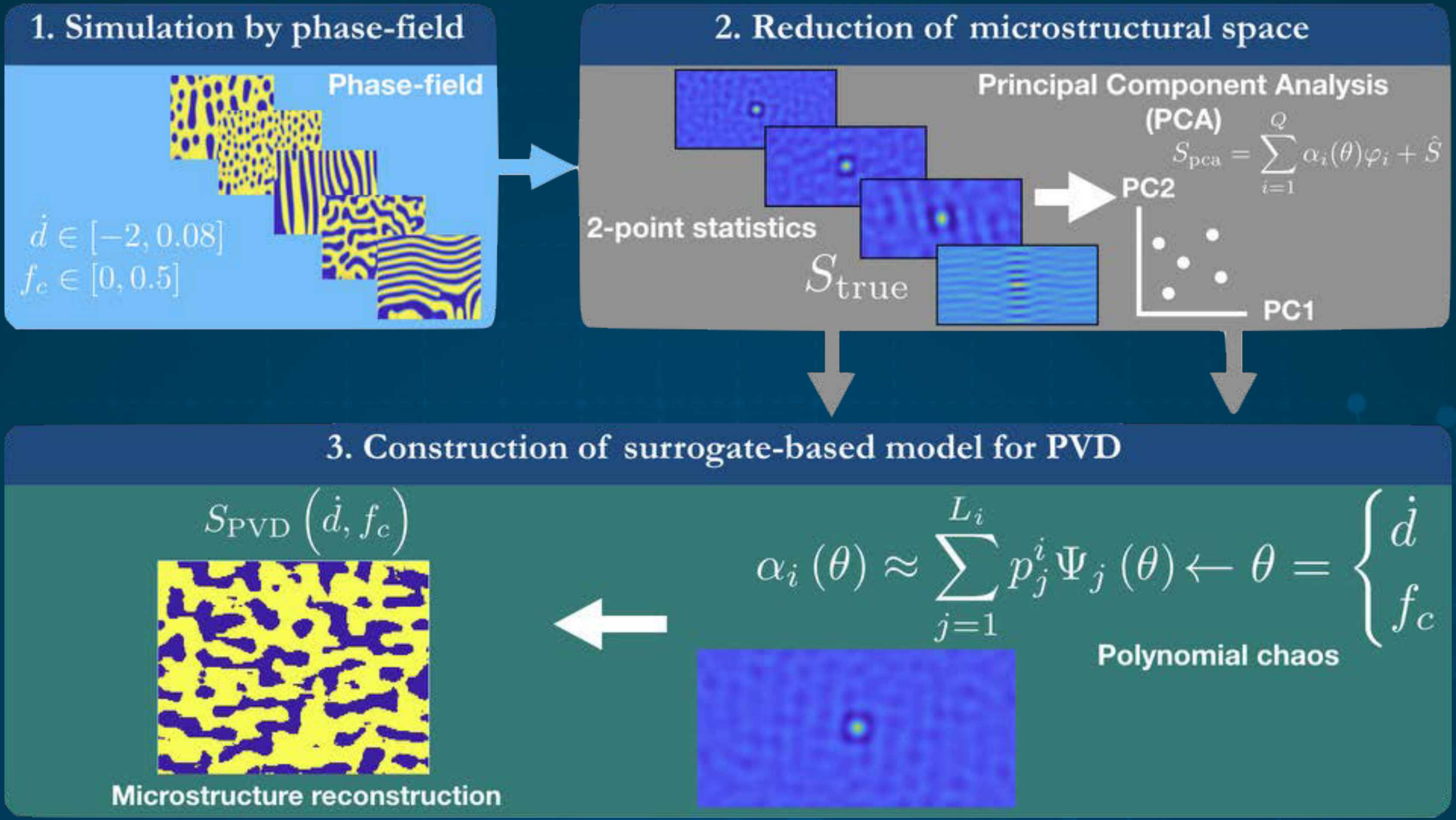


Fingerprint Of The Microstructure?

$$S_{pca}(\theta) = \sum_{I=1}^{Q} \alpha_i(\theta)\varphi_i + \hat{S}$$



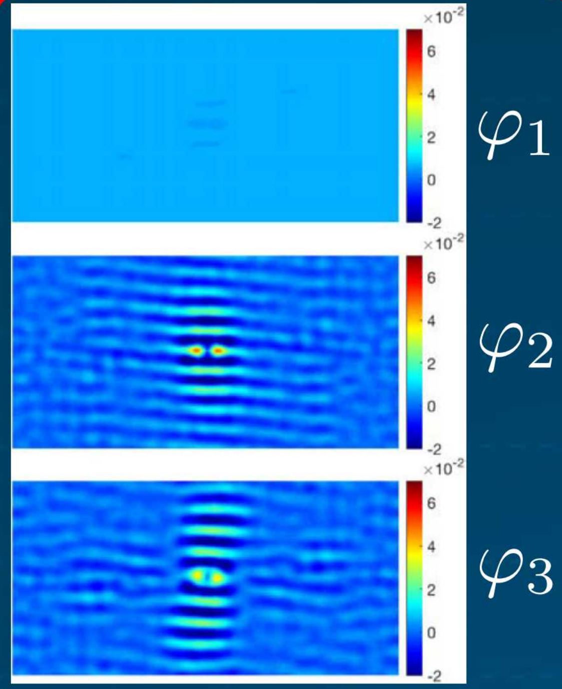
Rapidly Predicting Morphology?



Beyond Classical Regression?

PCA reduces the dimensionality

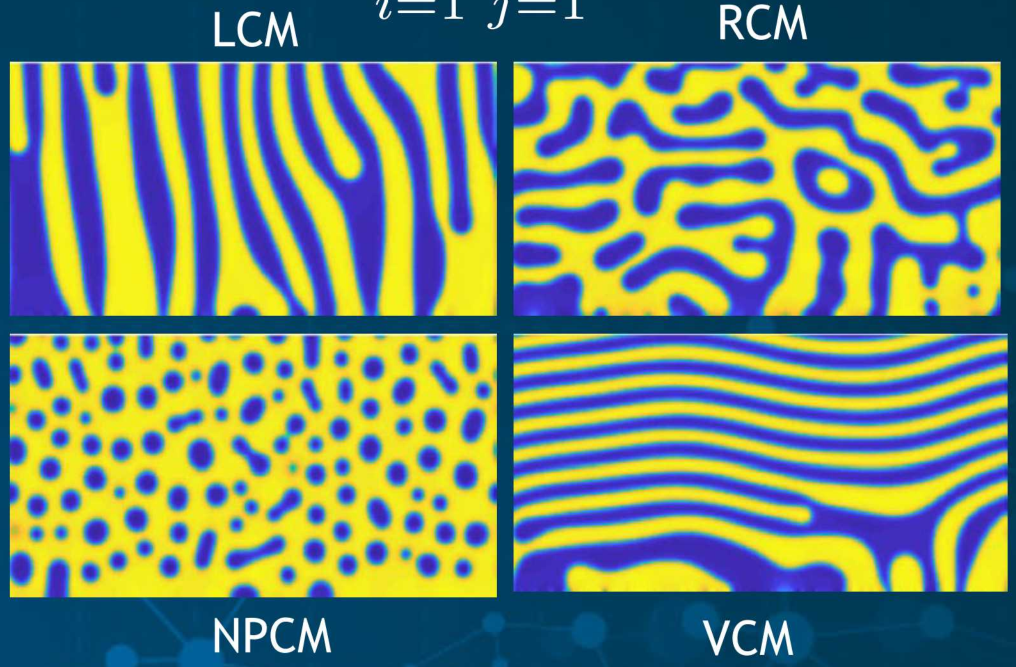
$$S_{\mathrm{pca}} = \sum_{i=1}^{Q} \alpha_i(\theta)\boxed{\varphi_i} + \hat{S}$$



Basis elements capture complexity of morphology and long-range correlations

PCE maps back to processing parameters

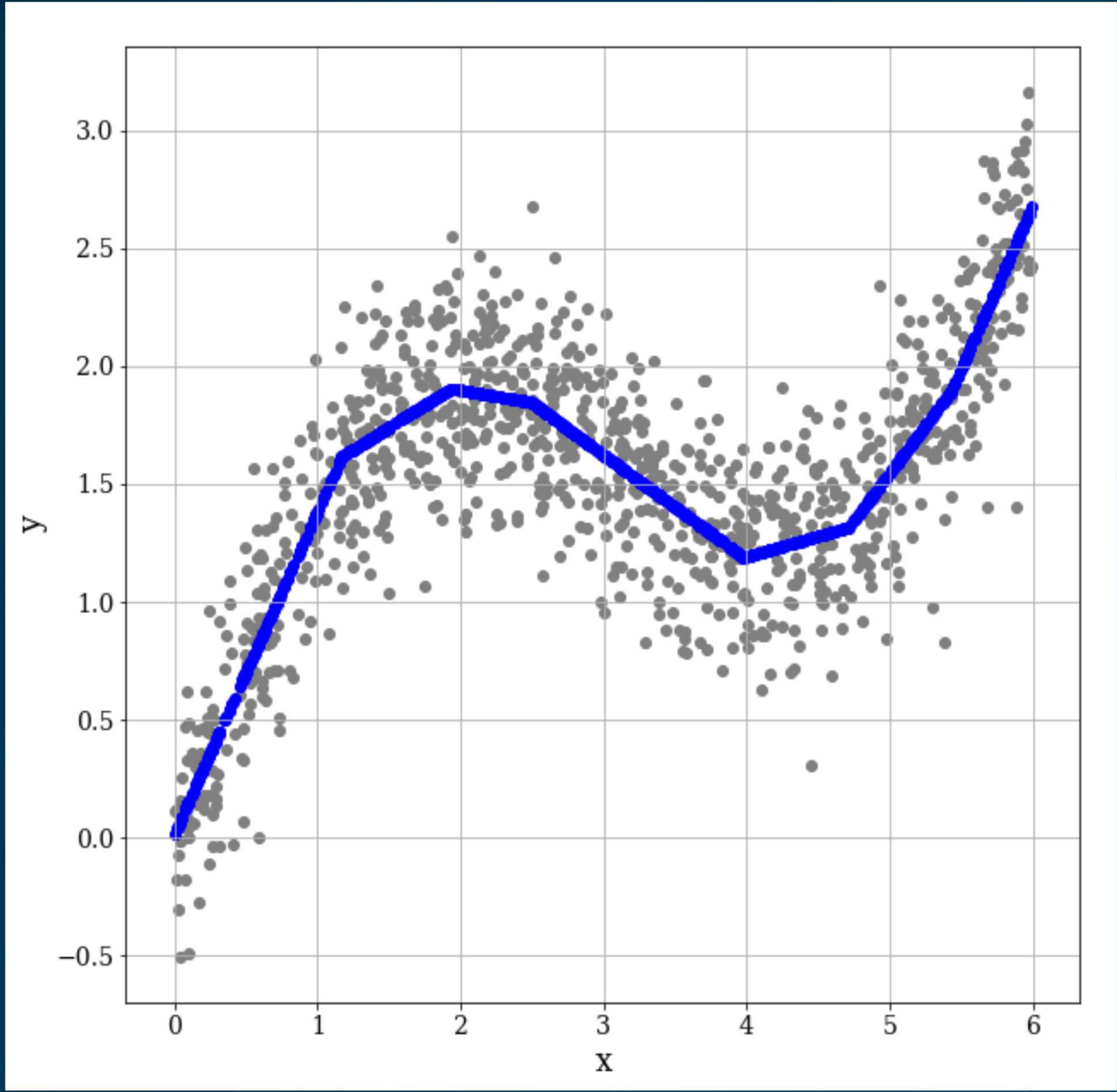
$$S_{\mathrm{predicted}} = \sum_{i=1}^{Q} \sum_{j=1}^{Li} p_j^i \Psi(\theta)\varphi_i + \hat{S}$$



Small changes in processing input space results in drastic changes in morphology: but…Legendre polynomial in PCE are continuous polynomials

Can We Leap in Time?

Time-series Forecasting



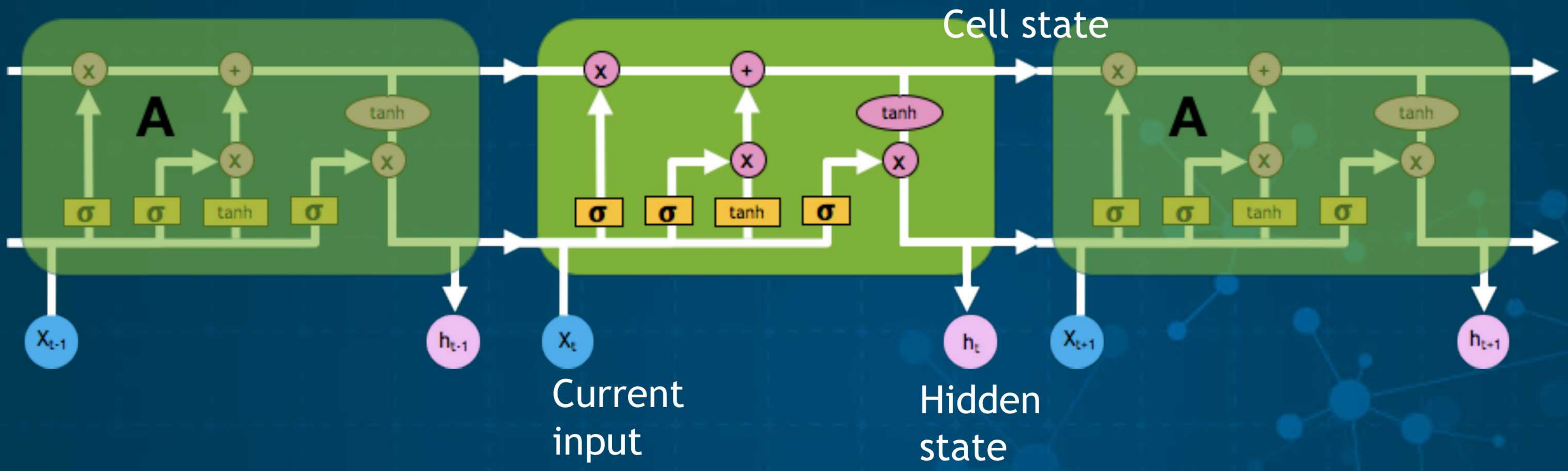
TIME-SERIES MULTIVARIATE ADAPTIVE REGRESSION SPLINES (TSMARS)

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,…

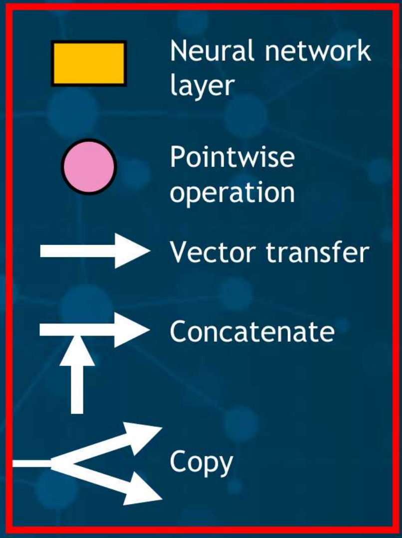
Time-series Forecasting

LONG SHORT TERM MEMORY NETWORK (LSTM)

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,…**

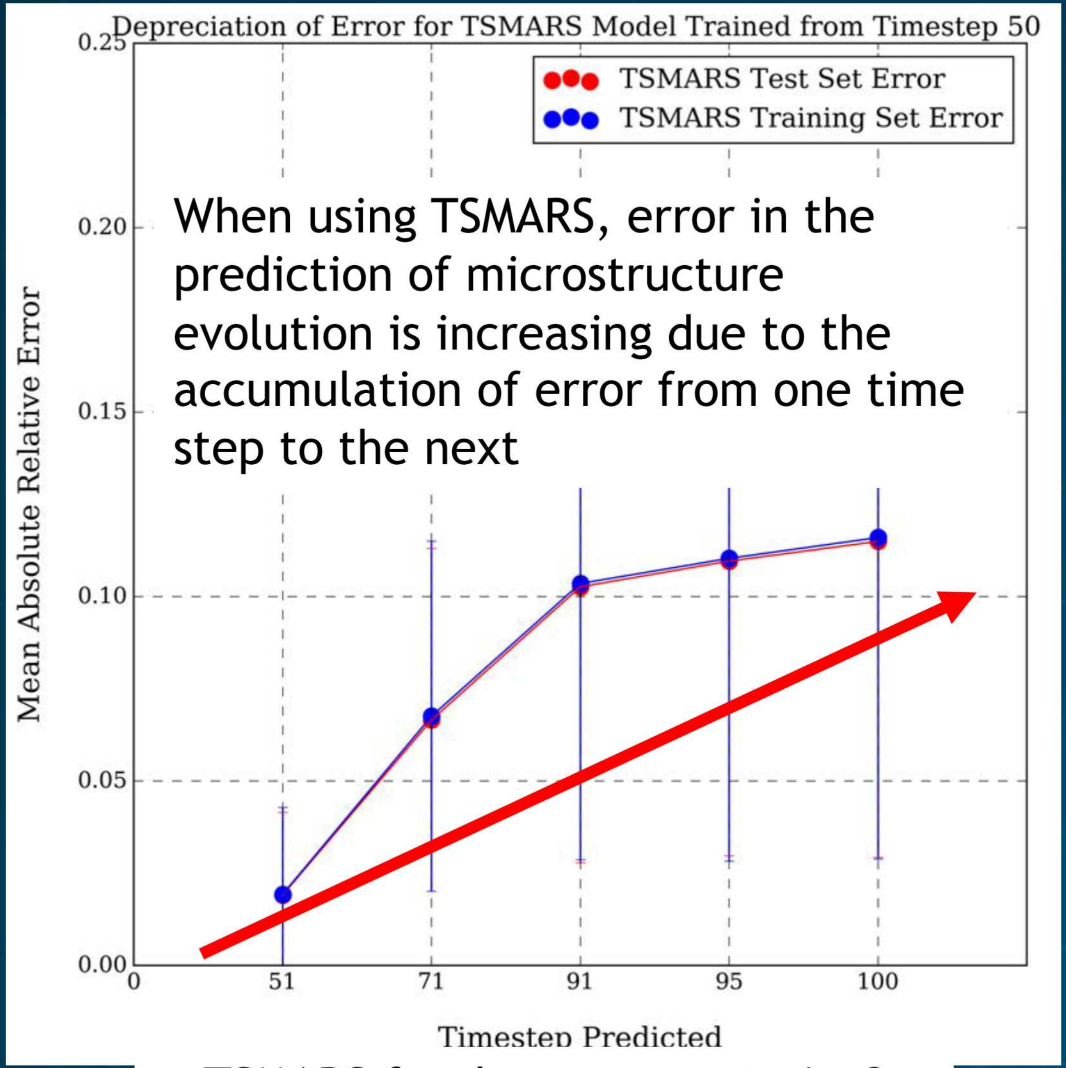


Nomenclature



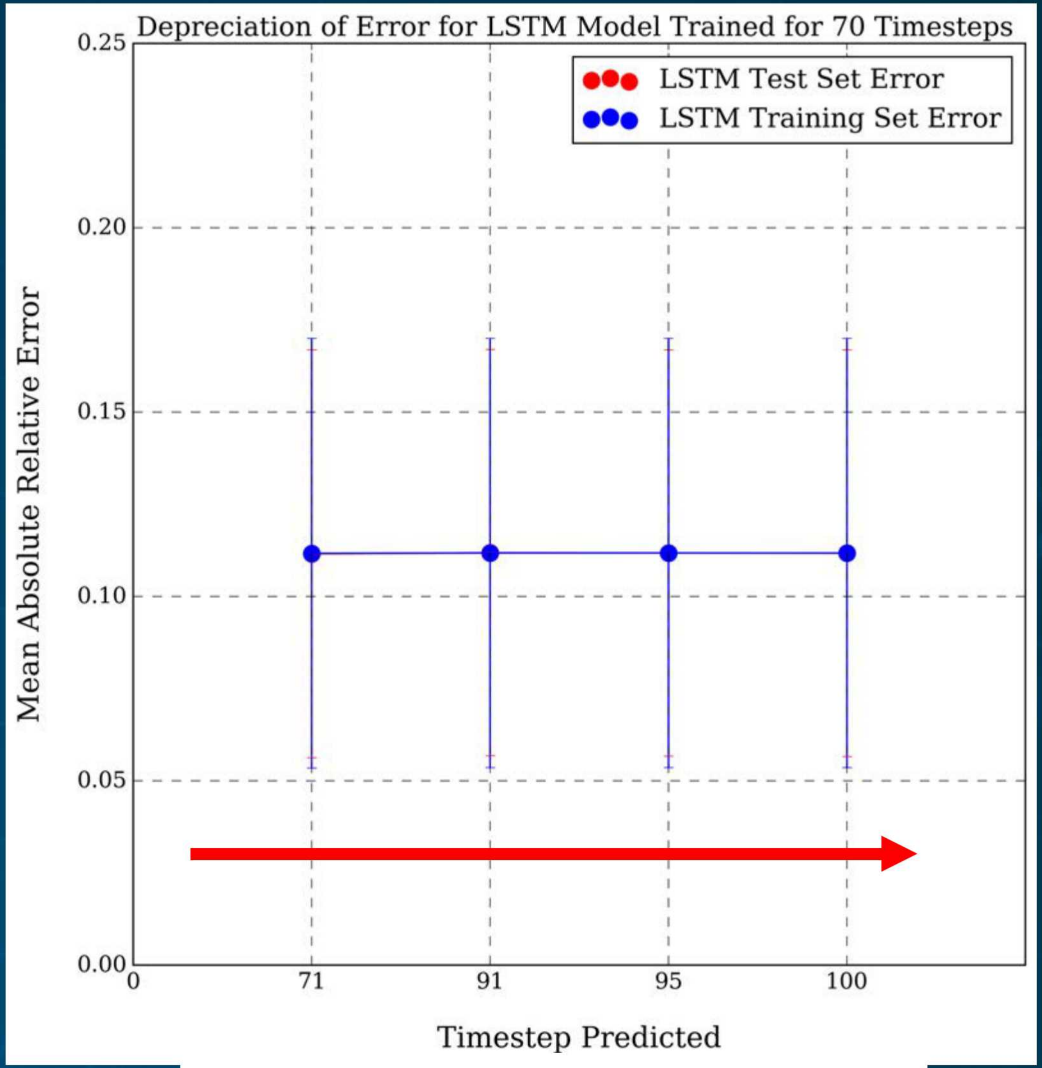
Why Do We Need A Deep Learning Strategy?

TSMARS



TSMARS for data augmentation?

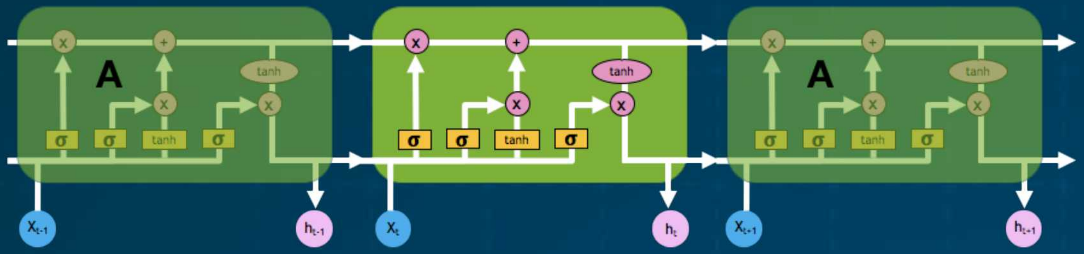
LSTM



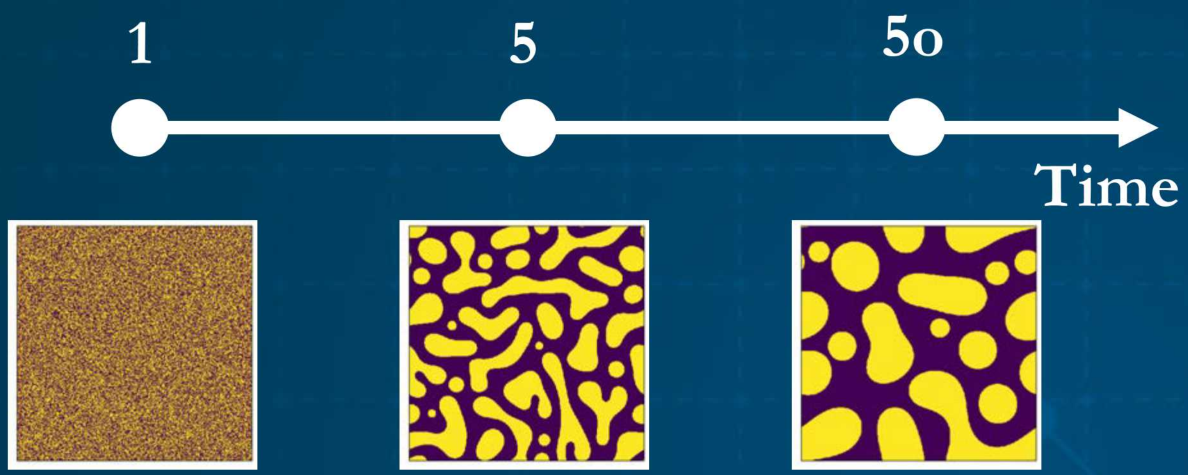
LSTM for PF acceleration?

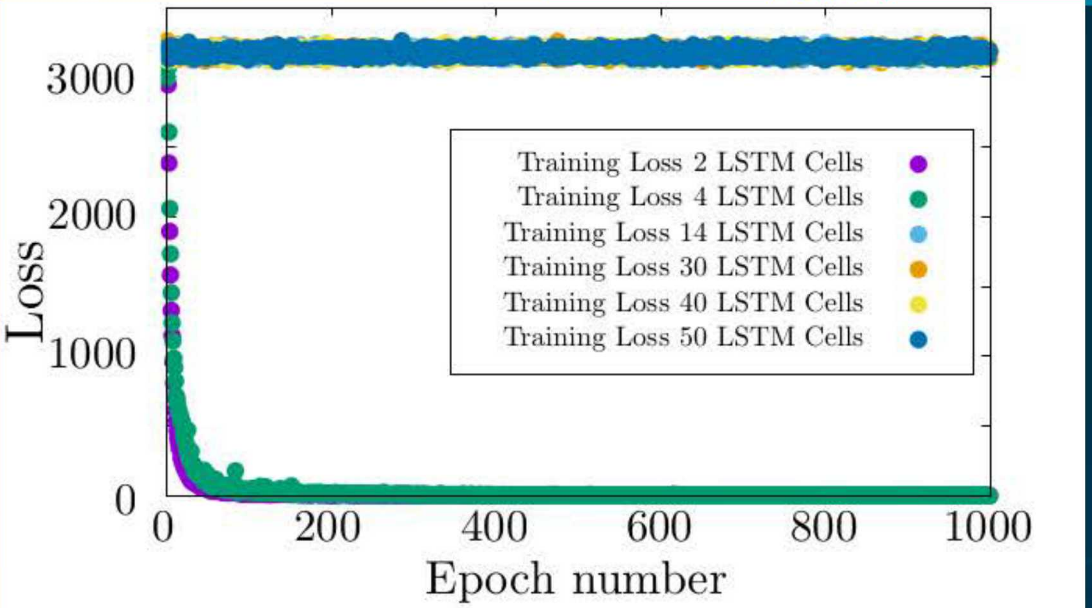
Optimum LSTM Architecture

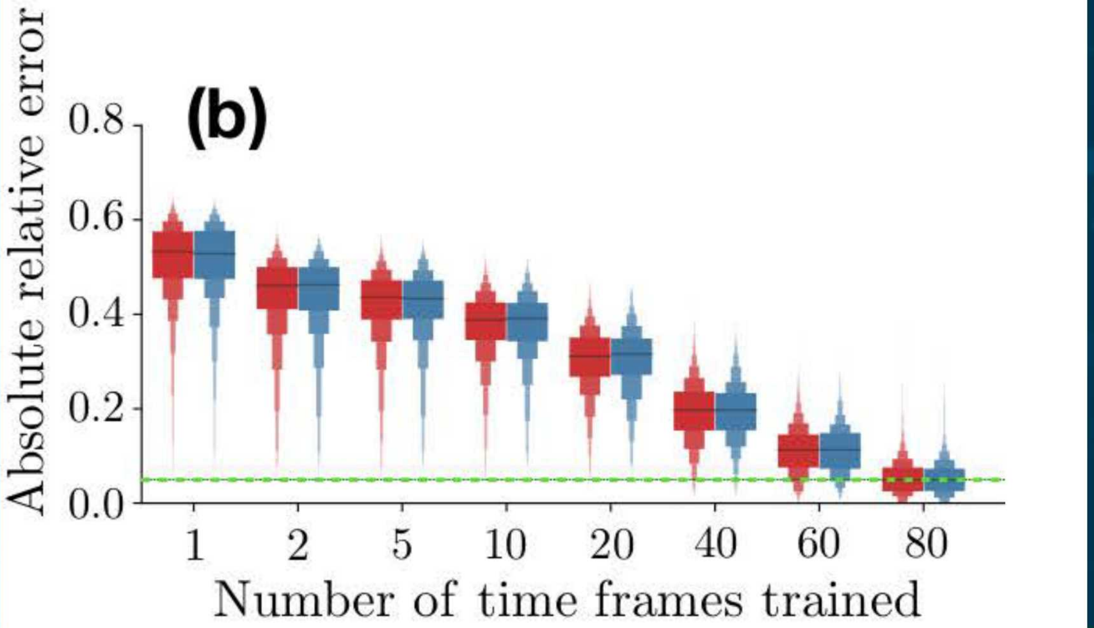
Number of LSTM cells:



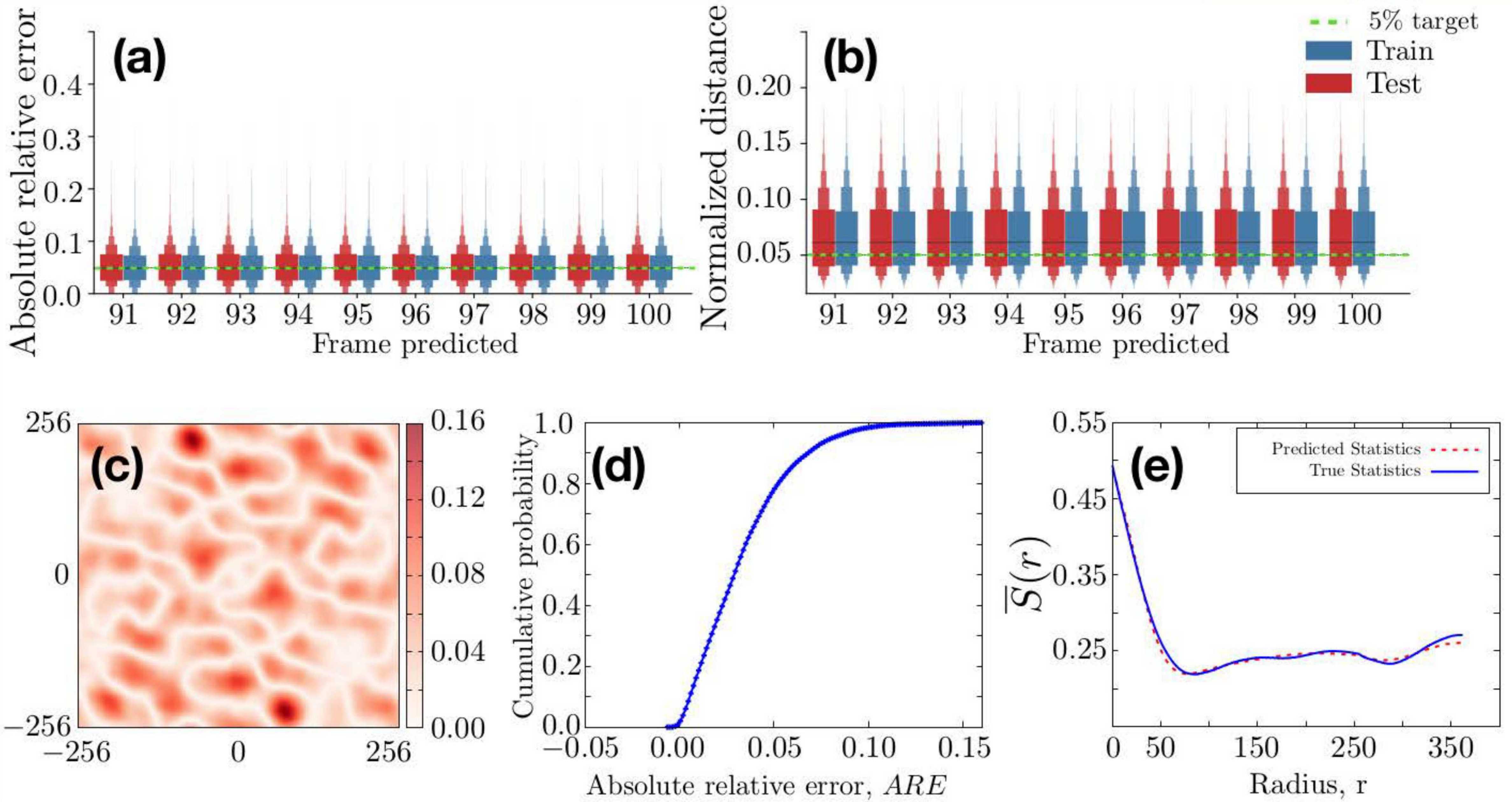
Number of time frames needed for training:





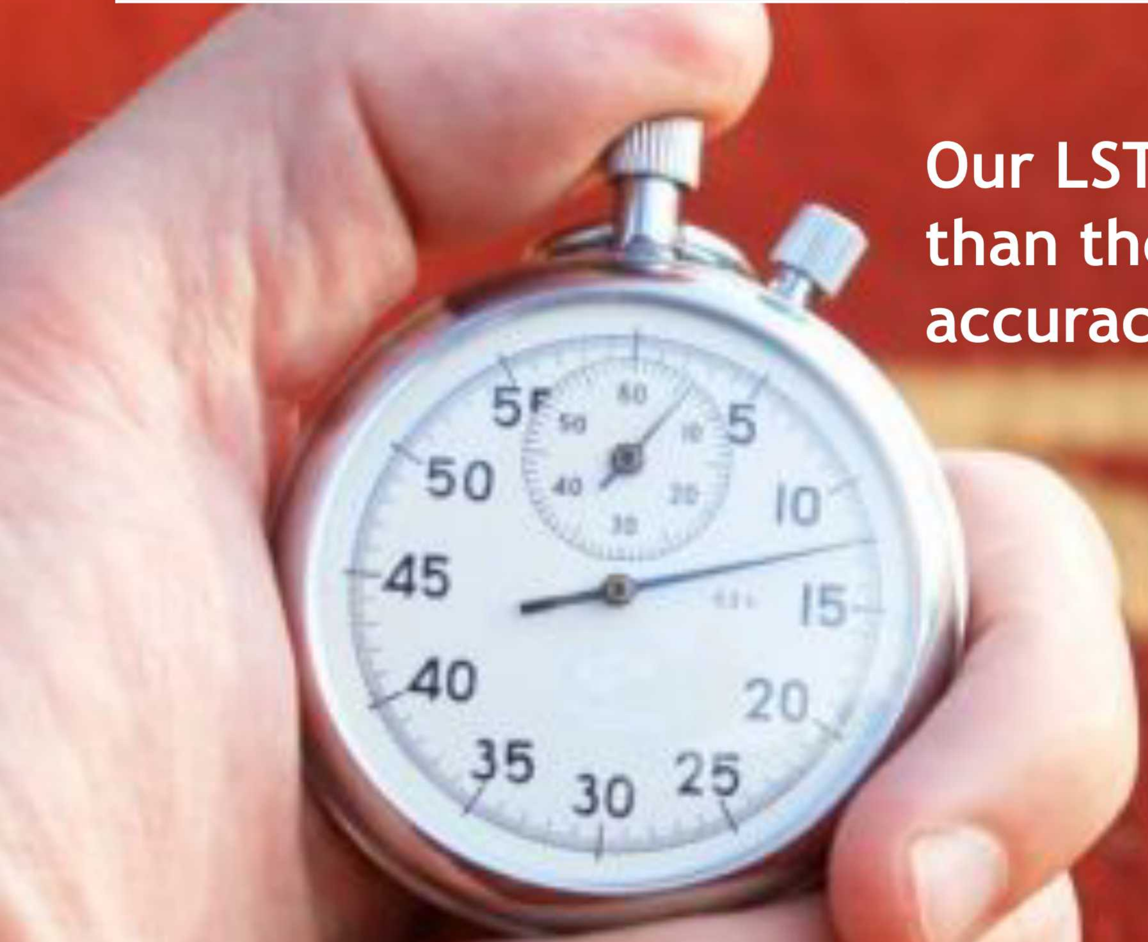


Performance of LSTM-Trained Model



Computational Efficiency

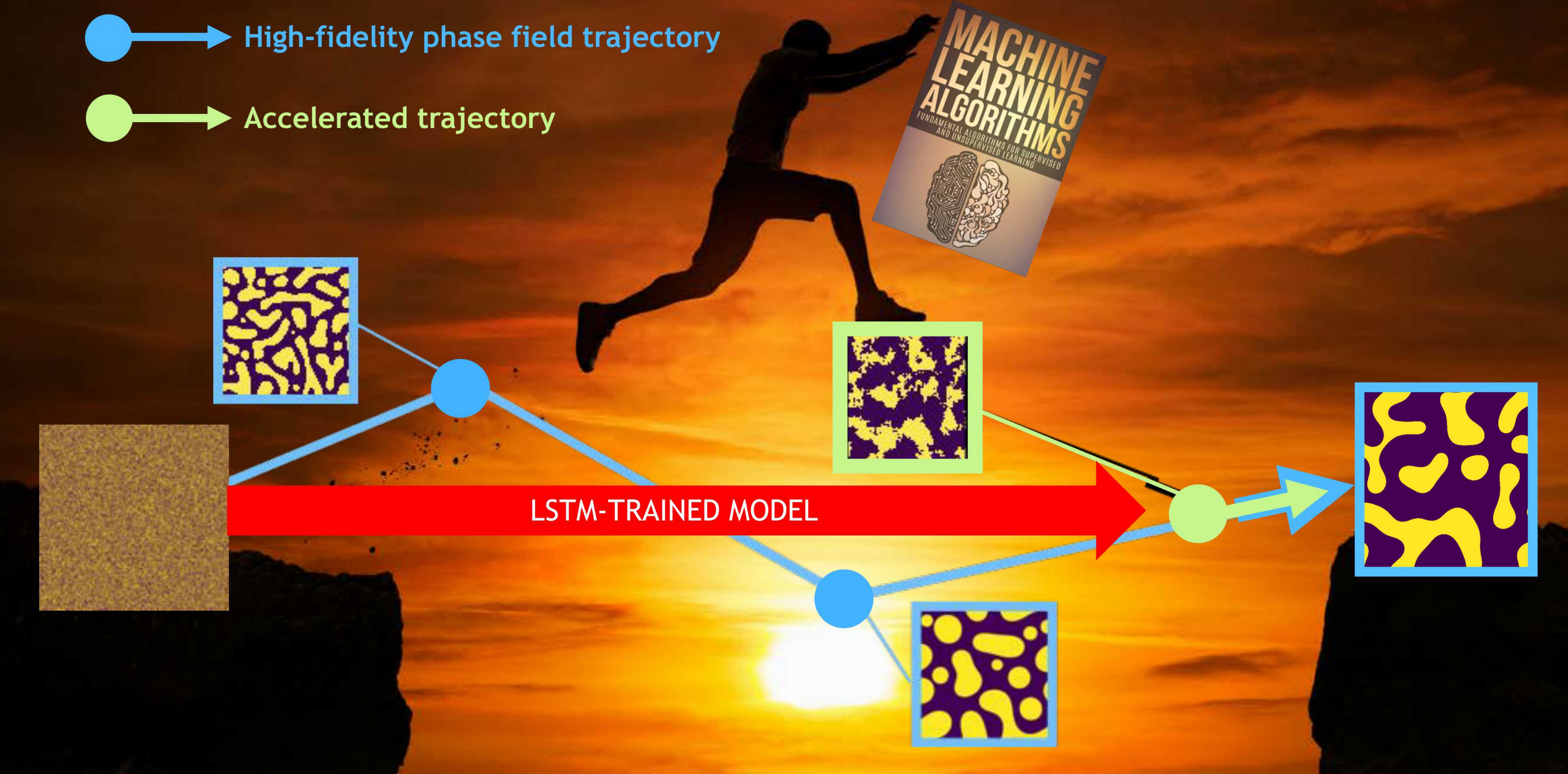
	High-fidelity	LSTM-trained
1 simulation for 5M time steps	96 mins	0.06s
50,000 simulations	~9 year and 1 month	50 mins



Our LSTM-trained framework is nearly 50,000 faster than the high-fidelity simulation with comparable accuracy!

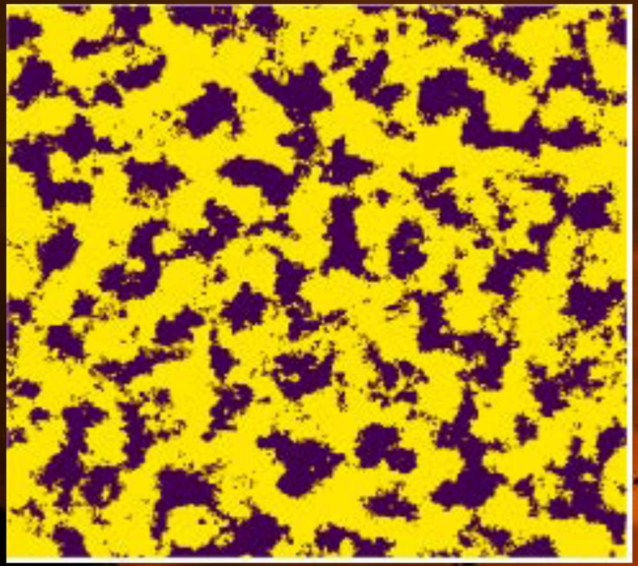
Opens a promising path forward for discovering, understanding and predicting evolutionary microstructural phenomena

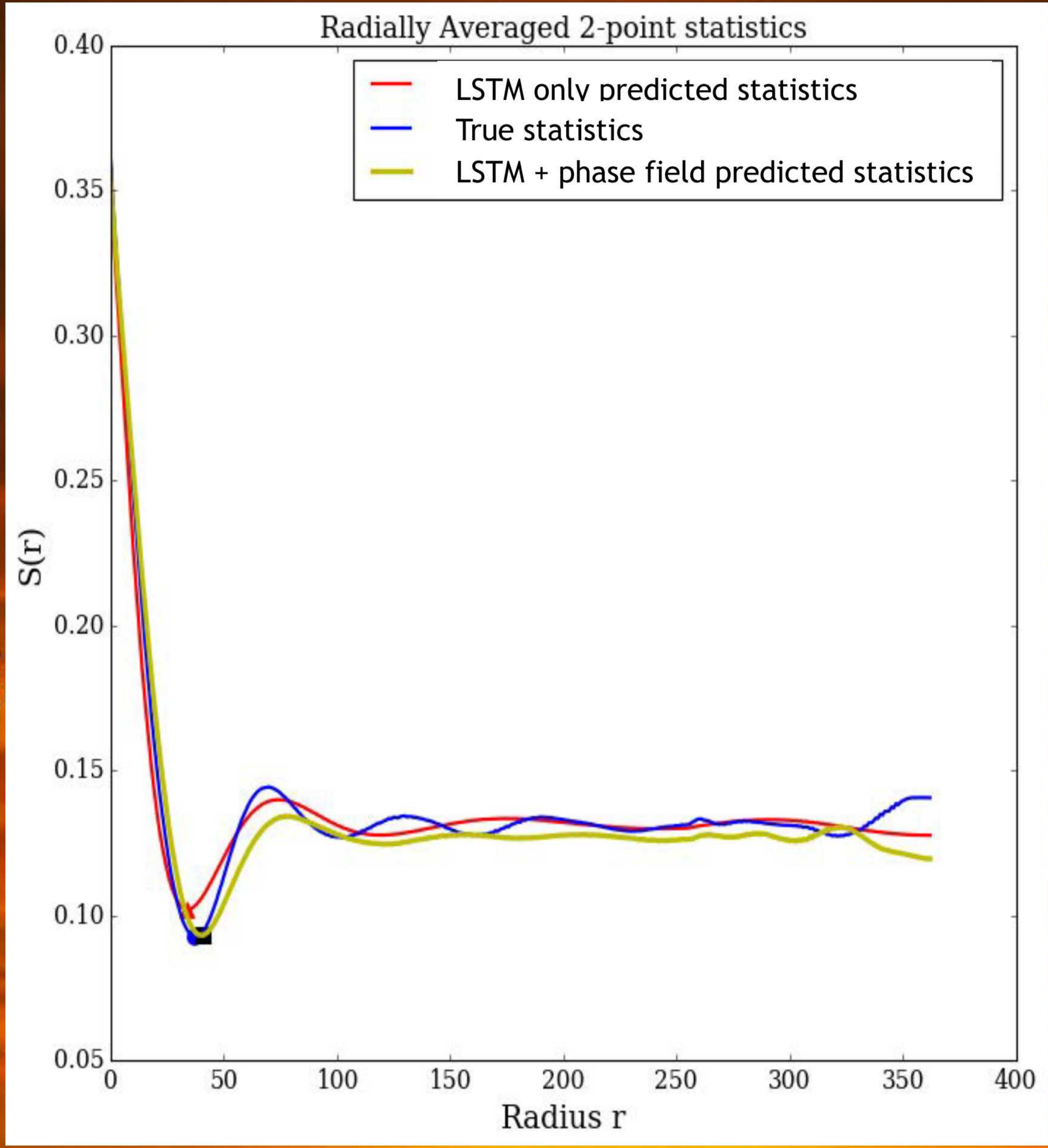
Accelerating Microstructure Evolution predictions: Leaping in Time Using Machine-learned Model



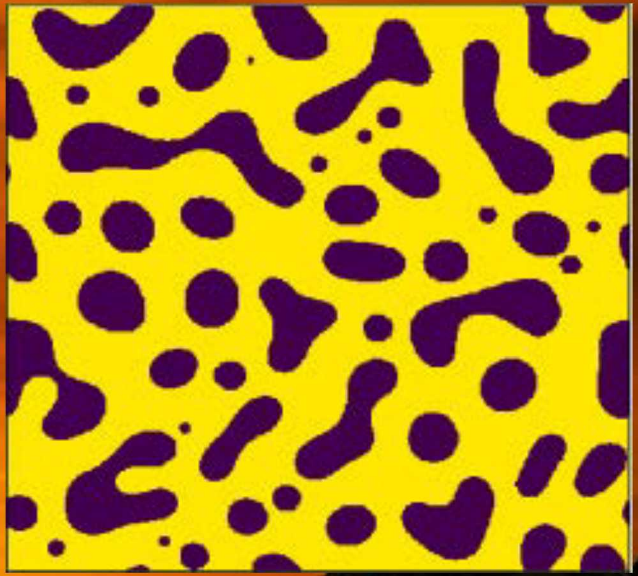
Accelerating Microstructure Evolution predictions: Leaping in Time Using Machine-learned Model

LSTM only



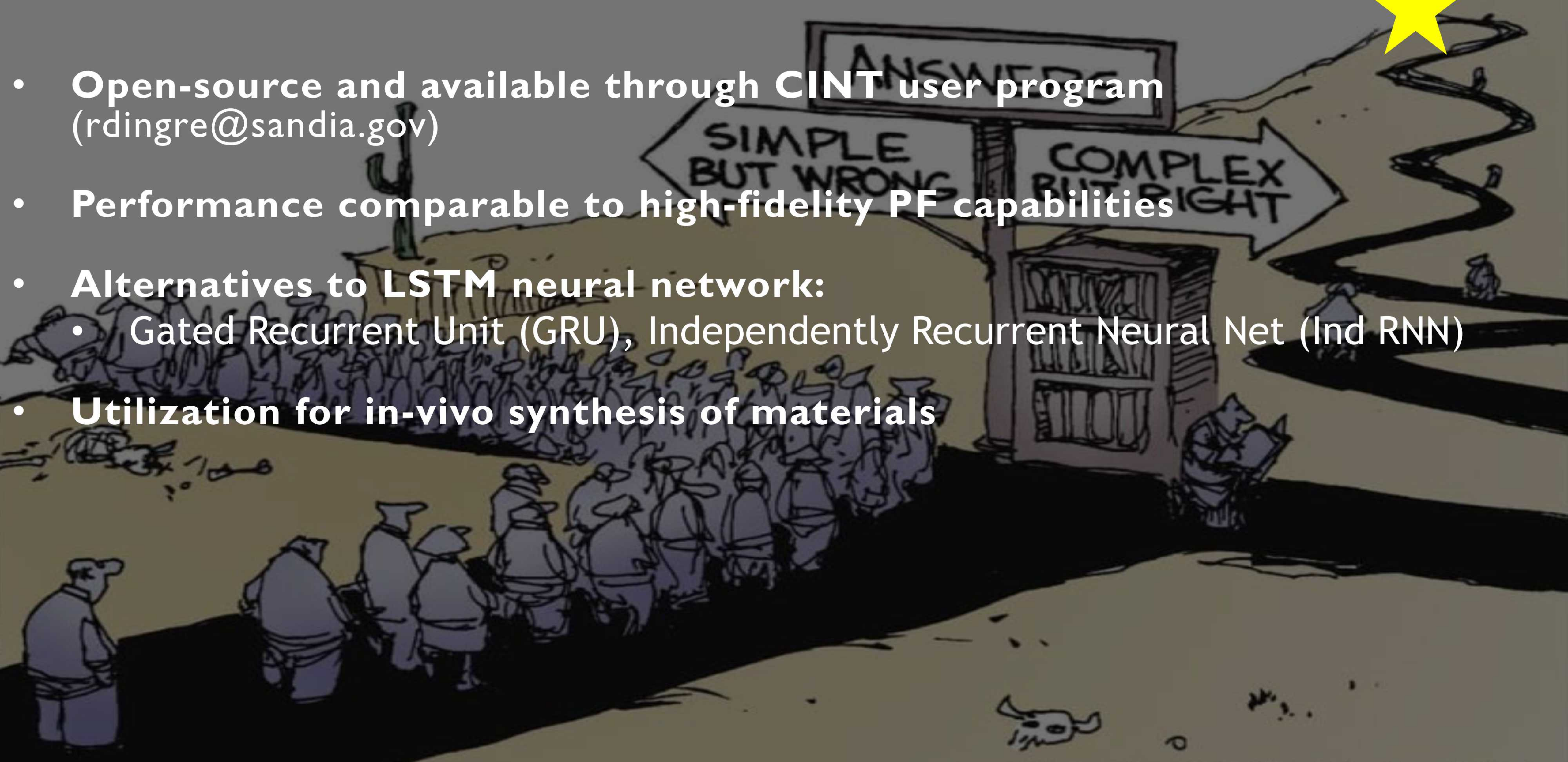


LSTM + phase-field



Moving Forward

- **Open-source and available through CINT user program** (rdingre@sandia.gov)
- **Performance comparable to high-fidelity PF capabilities**
- **Alternatives to LSTM neural network:**
  - Gated Recurrent Unit (GRU), Independently Recurrent Neural Net (Ind RNN)
- **Utilization for in-vivo synthesis of materials**



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