TMS ANNUAL MEETING 2022

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

David Montes De Oca Zapiain, Chongze Hu, Shawn Martin, James stewart, Rémi Dingreville

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Predicting Microstructure Evolution Via Phase-Field

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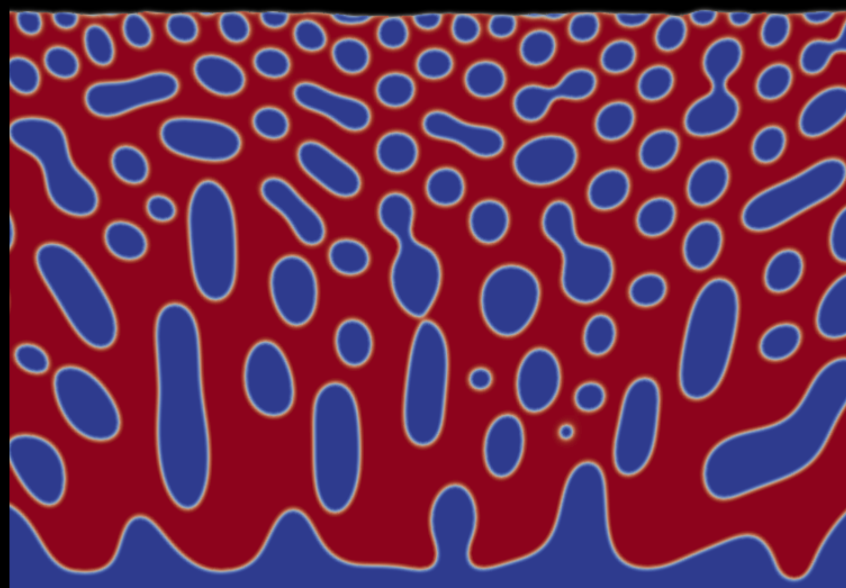
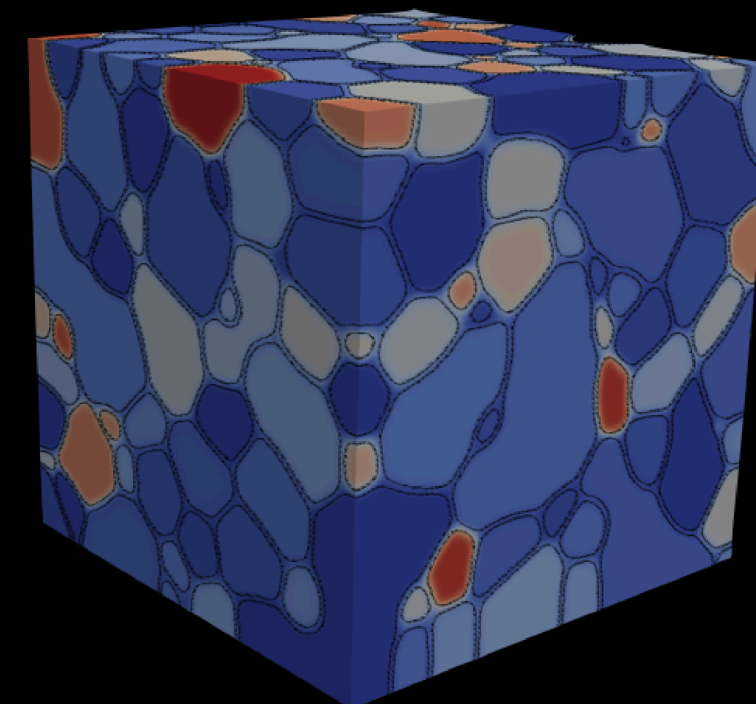
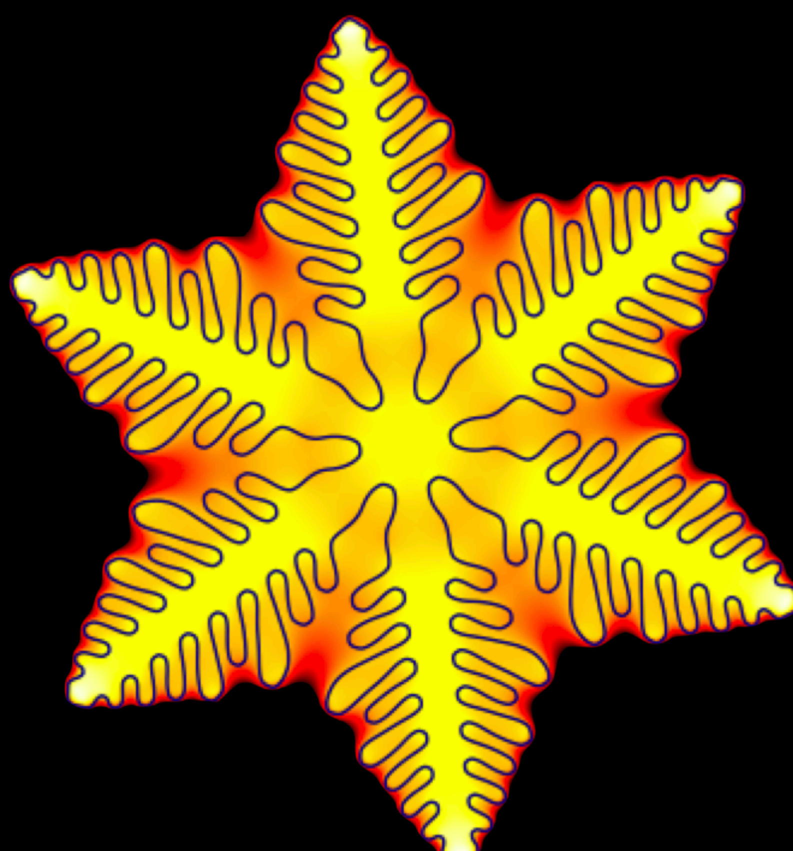
Physical Vapor Deposition

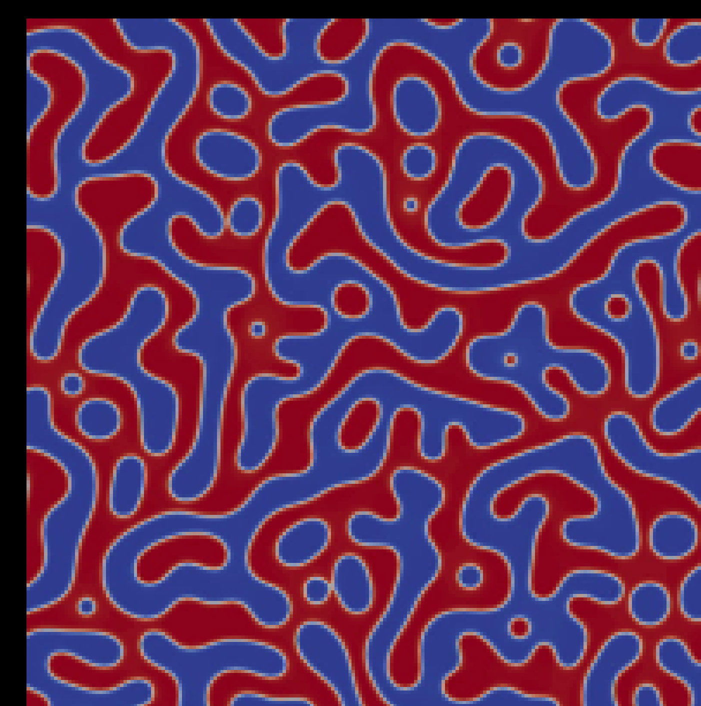


Grain Growth





Solidification



Phase Separation

Learn How to Trigger Microstructure Formation Mechanisms on Demand

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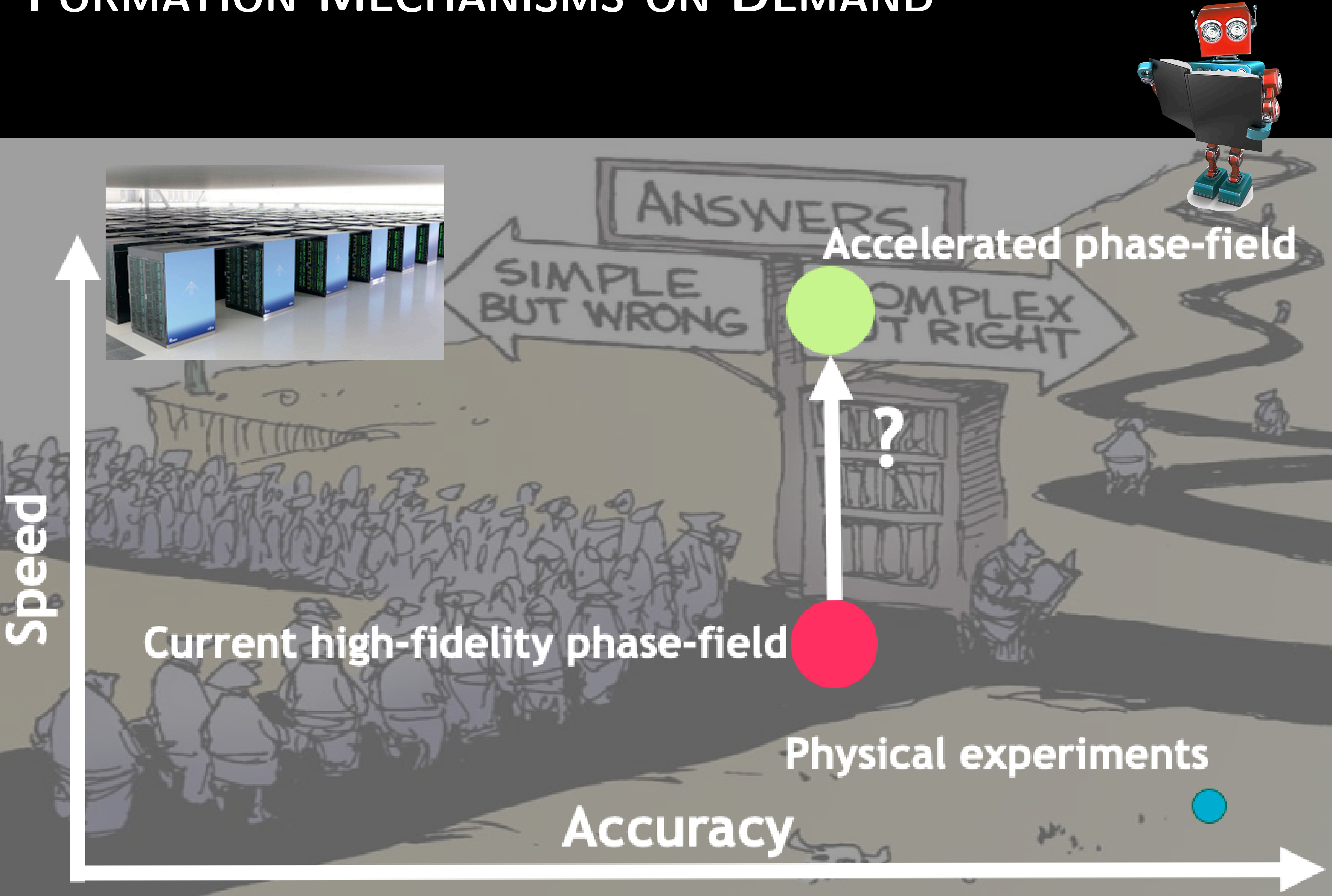

We Can Map Process To Structure Using Dimensionality Reduction and Polynomial Chaos Expansion

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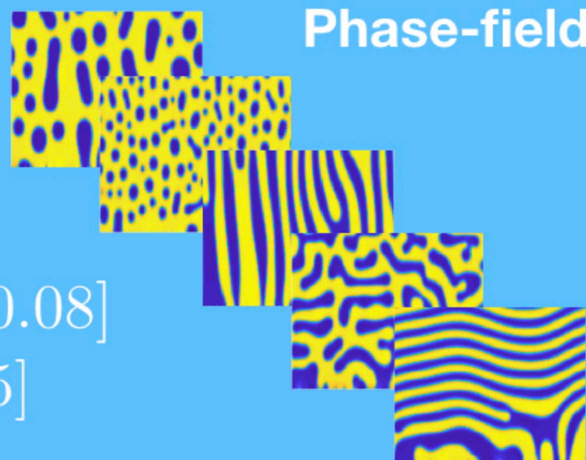
1. Simulation by phase-field

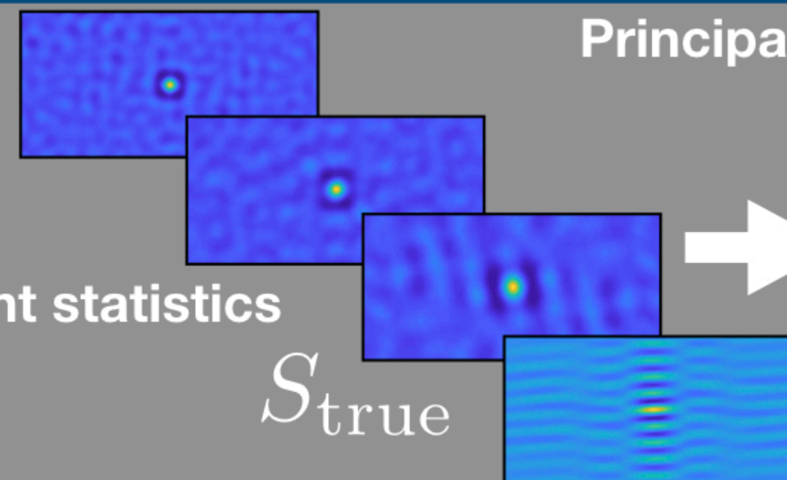
Phase-field



$\dot{d} \in [-2, 0.08]$

$f_c \in [0, 0.5]$

2. Reduction of microstructural space



2-point statistics

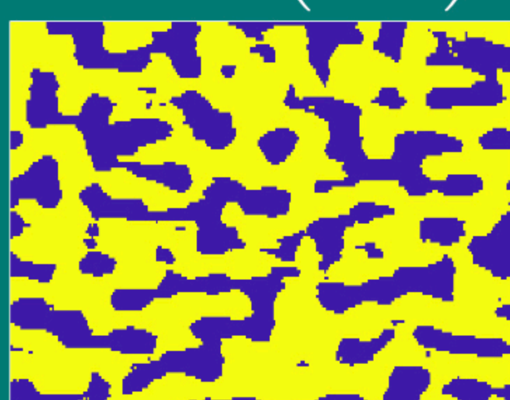
S_{true}

Principal Component Analysis (PCA)

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

3. Construction of surrogate-based model for PVD

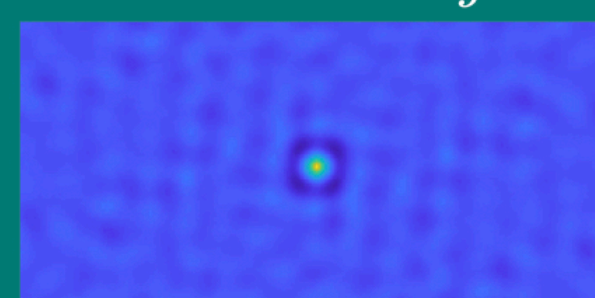
$S_{\text{PVD}}\left(\dot{d}, f_c\right)$



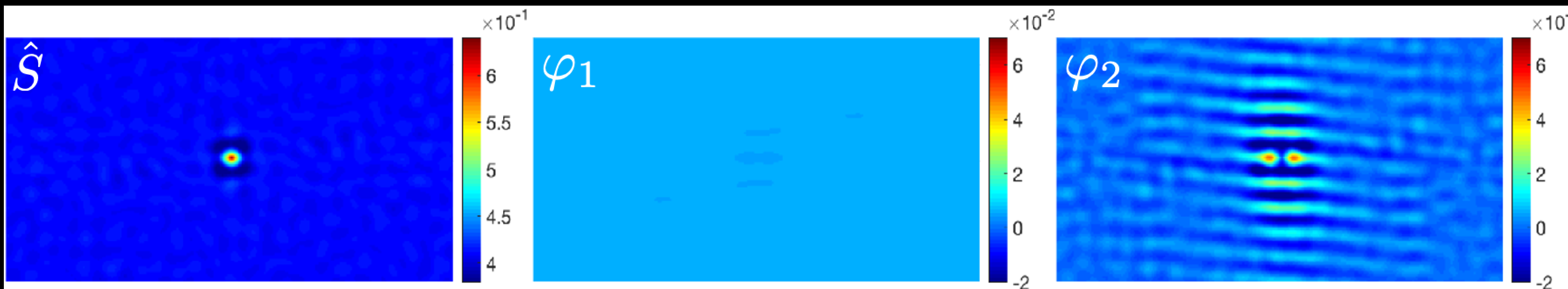
Microstructure reconstruction

$$\alpha_i(\theta) \approx \sum_{j=1}^{L_i} p_j^i \Psi_j(\theta) \leftarrow \theta = \begin{cases} \dot{d} \\ f_c \end{cases}$$

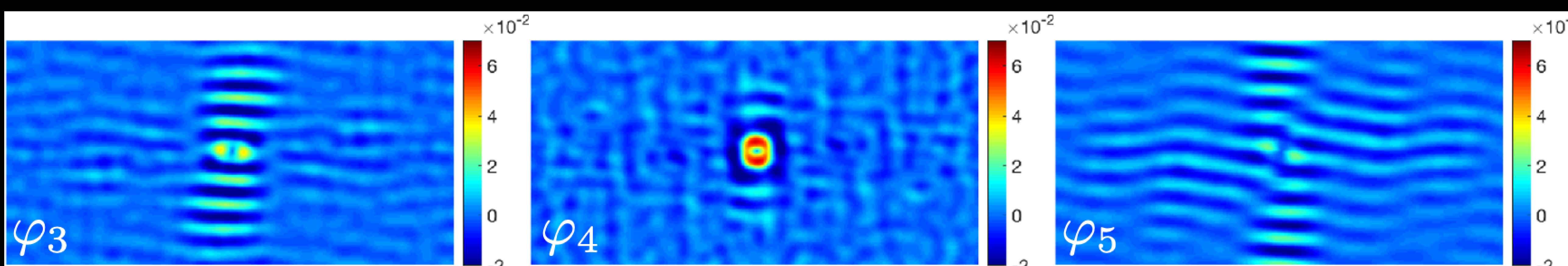
Polynomial chaos



Fingerprinting of the Microstructure: Capturing Short and Long Range Salient Features



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



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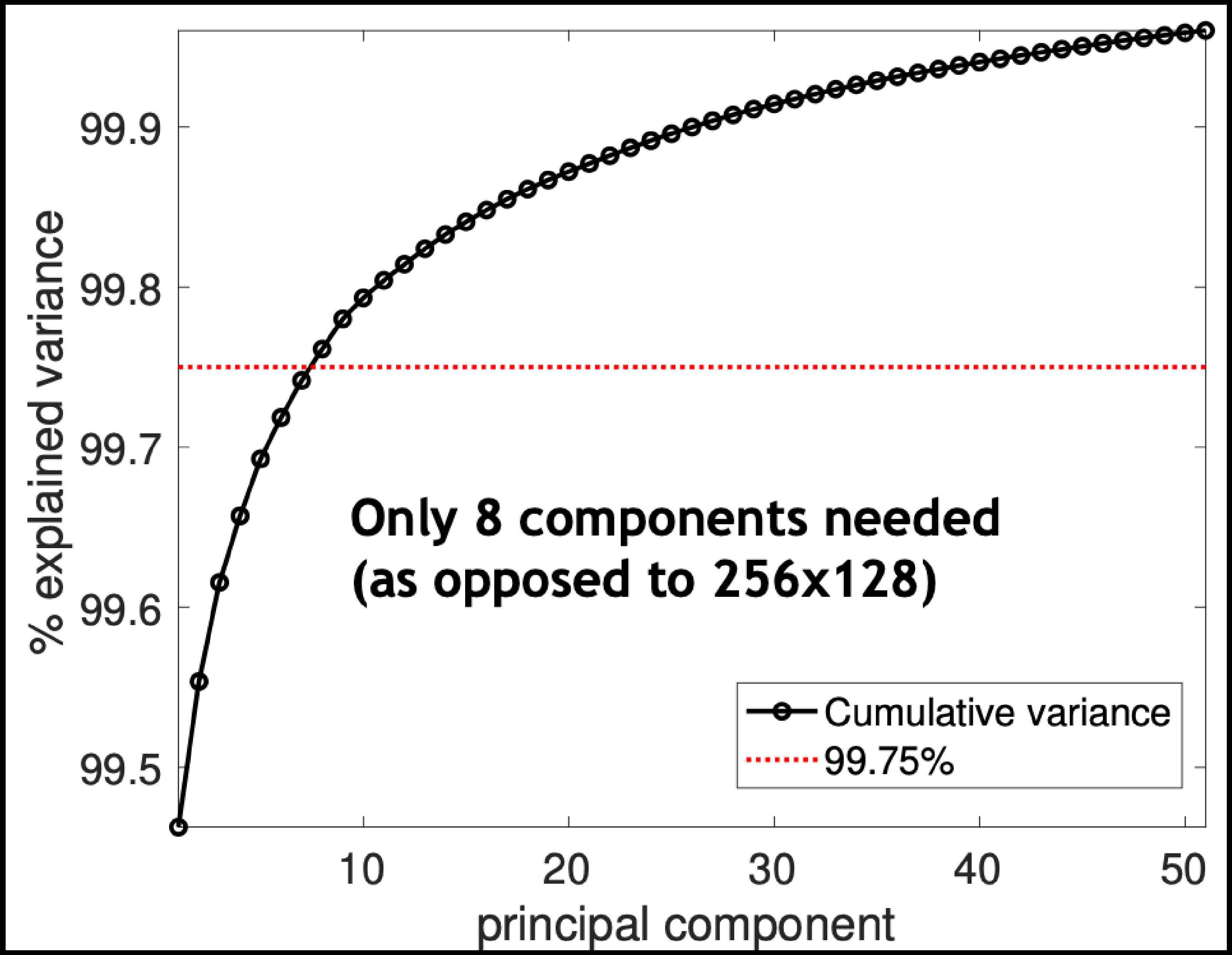
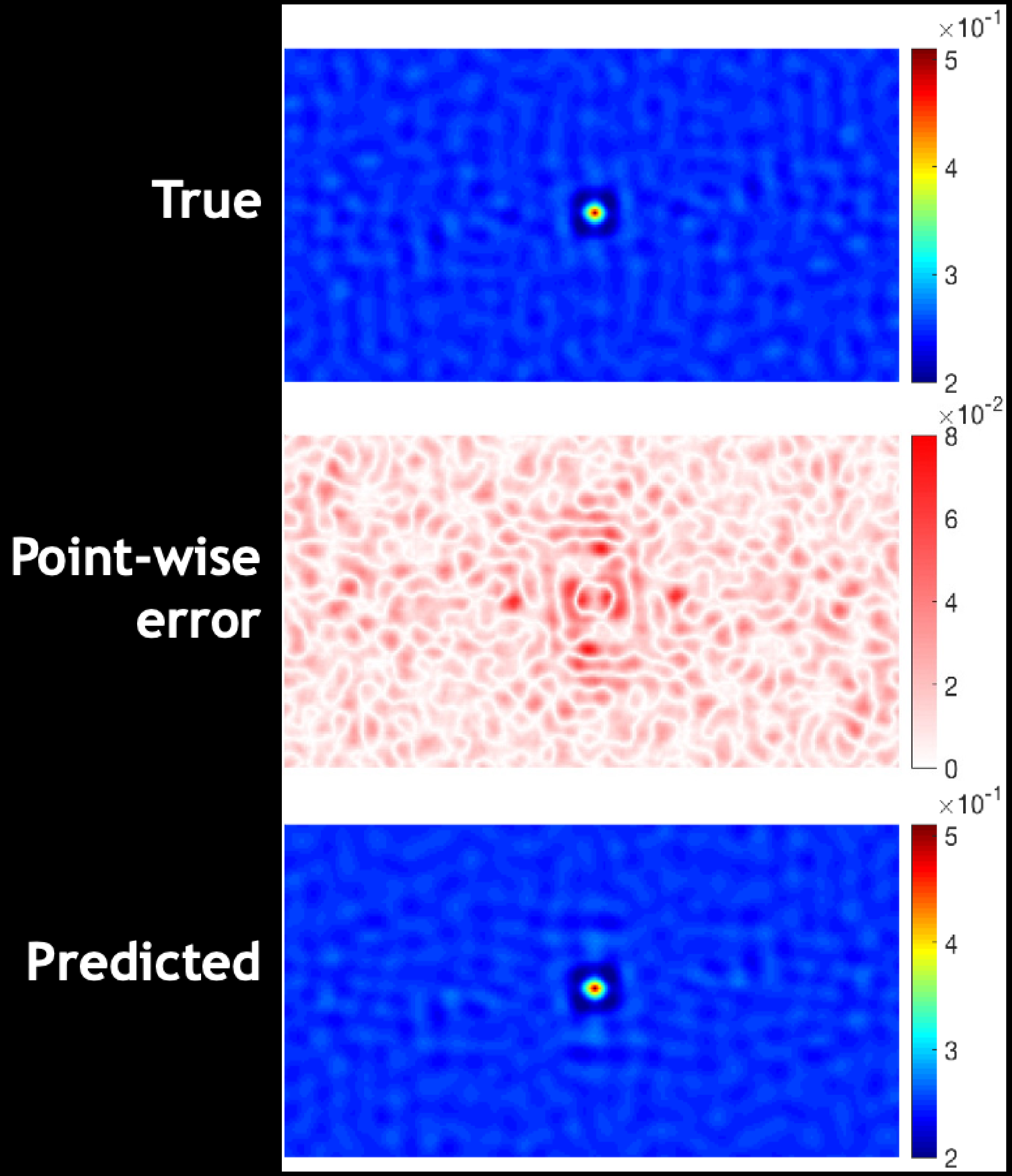
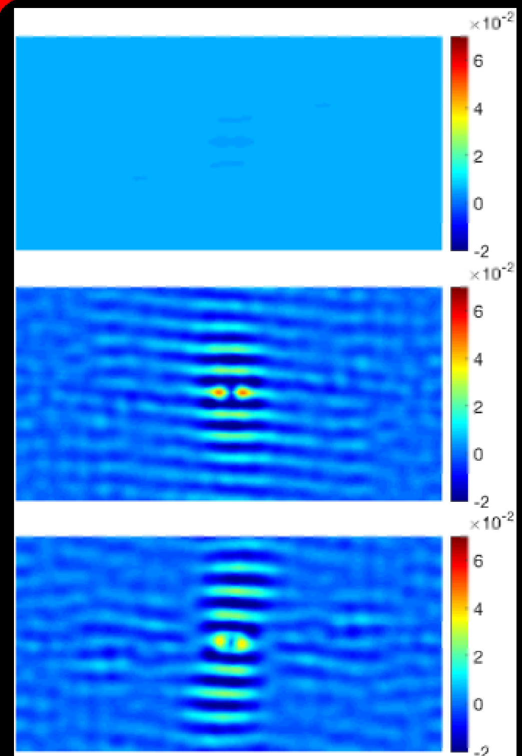




Sources of Errors Come From Both Steps

PCA reduces the dimensionality

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



φ_1

φ_2

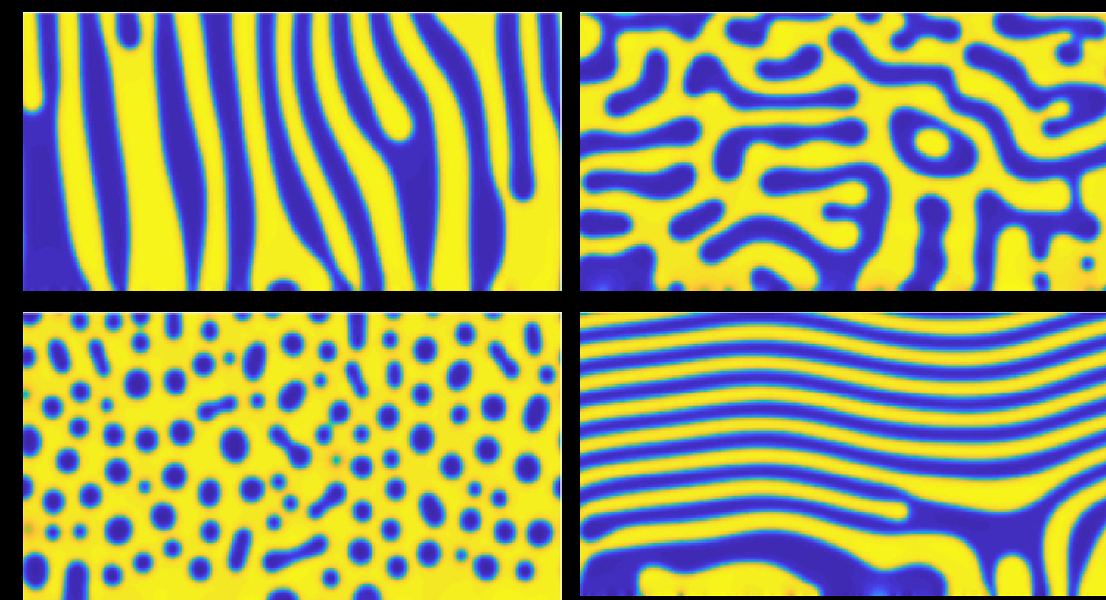
φ_3

Basis elements capture complexity of morphology and long-range correlations

PCE maps back to processing parameters

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

LCM RCM



NPCM VCM

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

Error	min	max	mean	standard deviation
$\mathrm{err}_1\ (\boldsymbol{\theta}_{\mathrm{train}})$	0.0030	0.0690	0.0146	0.0123
$\mathrm{err}_1\ (\boldsymbol{\theta}_{\mathrm{test}})$	0.0030	0.0441	0.0123	0.0091

err_1: Error on 2pt-stats: true vs. predicted

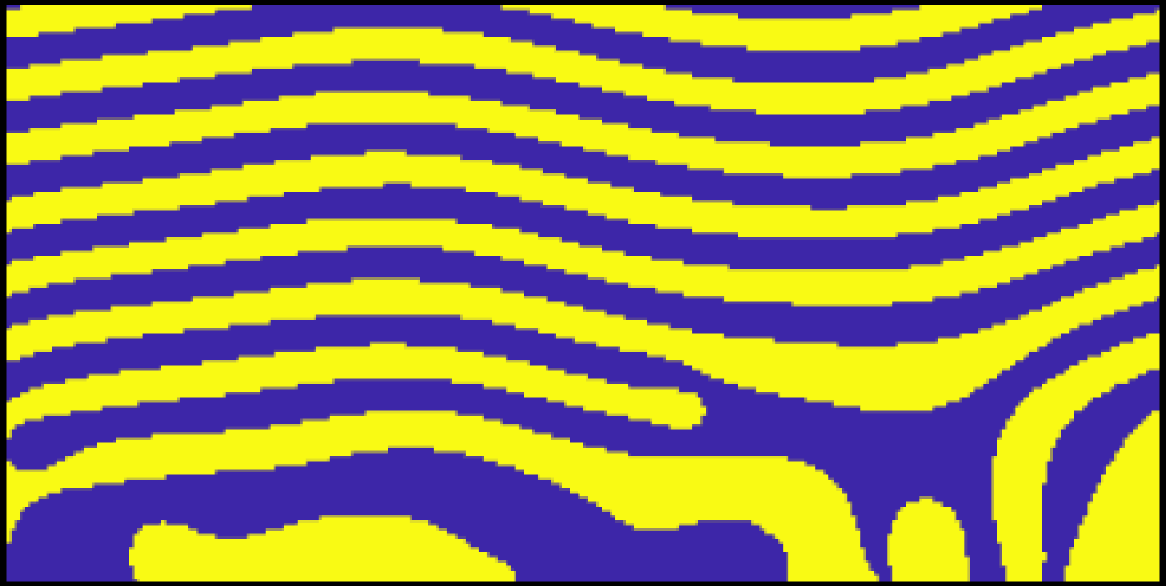
<

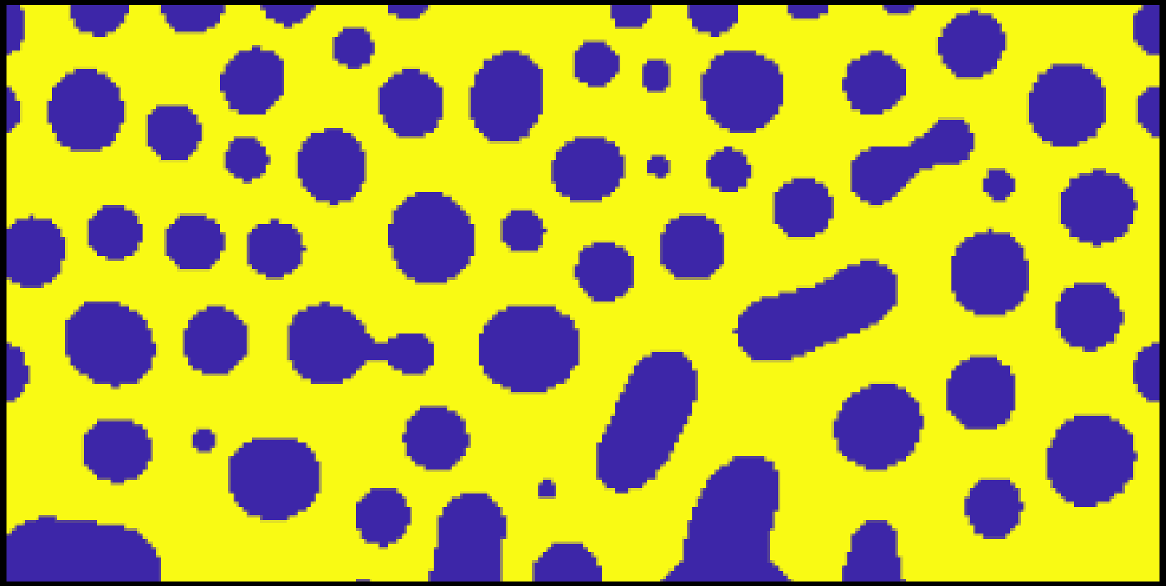
Error	min	max	mean	standard deviation
$\mathrm{err}_2\ (\boldsymbol{\theta}_{\mathrm{train}})$	0.0920	5.7683	0.8109	1.0067
$\mathrm{err}_2\ (\boldsymbol{\theta}_{\mathrm{test}})$	0.1106	2.8706	0.5296	0.5065
$\mathrm{err}_3\ (\boldsymbol{\theta}_{\mathrm{train}})$	0.0032	0.1197	0.0206	0.0223
$\mathrm{err}_3\ (\boldsymbol{\theta}_{\mathrm{test}})$	0.0032	0.0771	0.0154	0.0139

err_2: Error on PC scores

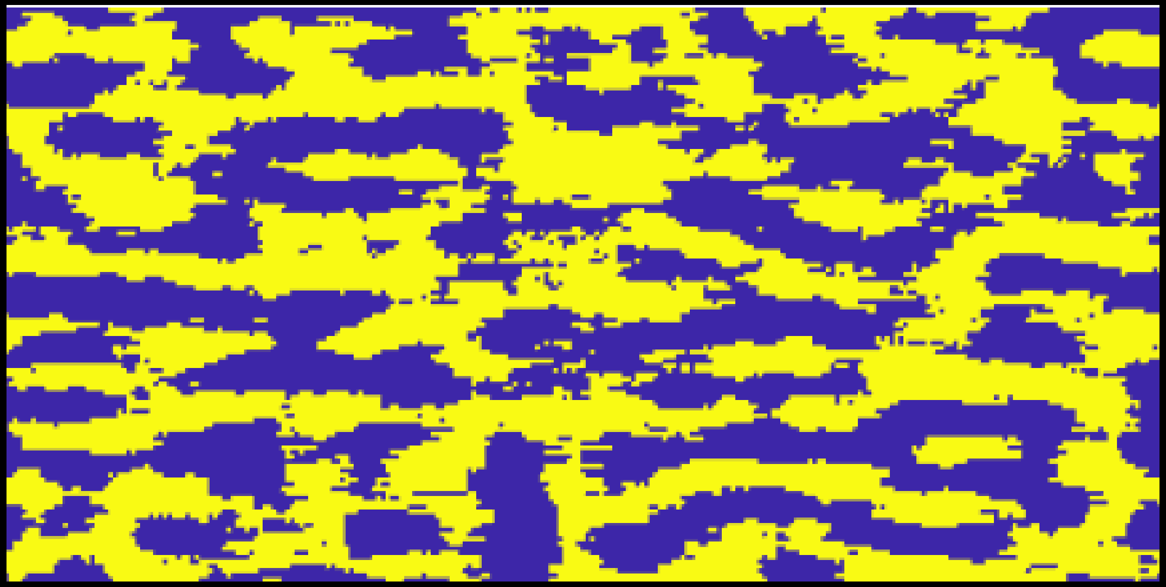
err_3: Error on 2pt-stats: true vs. predicted

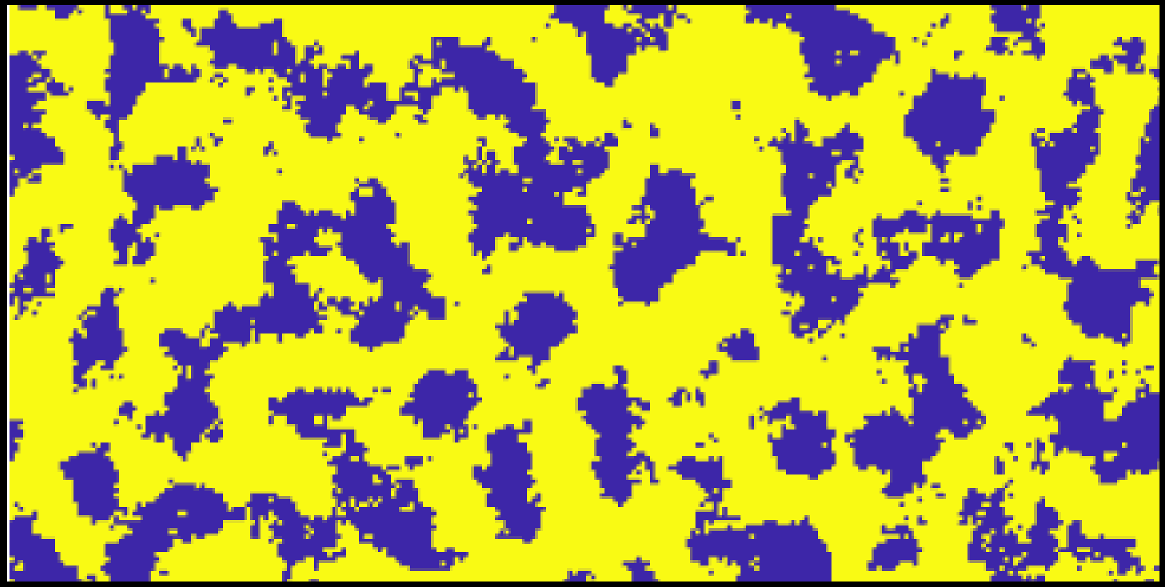
Comparison between True and Predicted Microstructures...Some Information is Lost





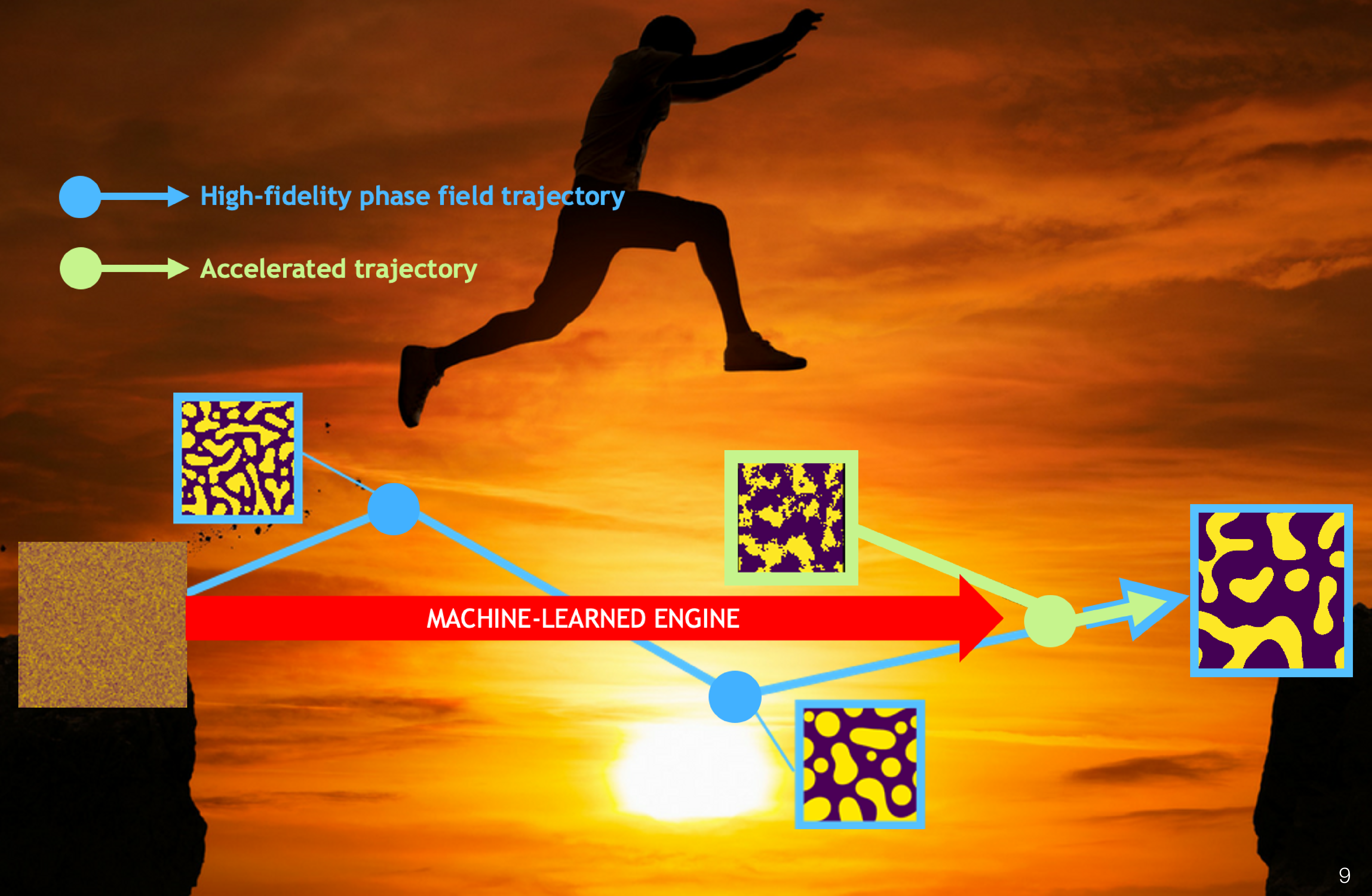
Reconstruction from surrogate model





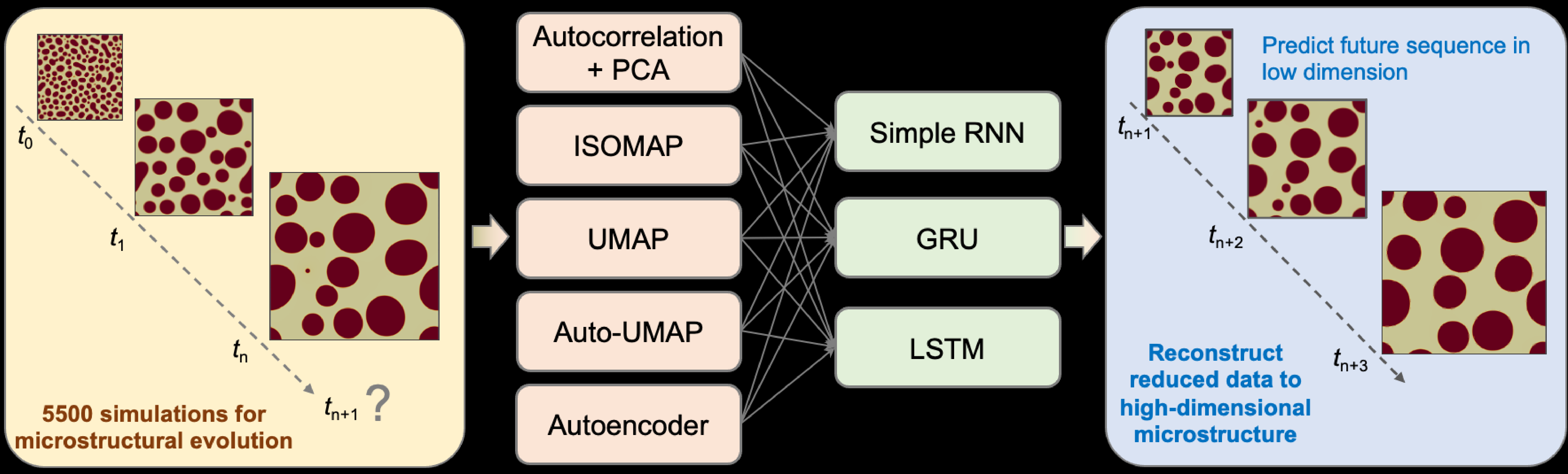
Can we Leap In Time Instead?

Reframing Microstructure Evolution as a Multivariate Time Series

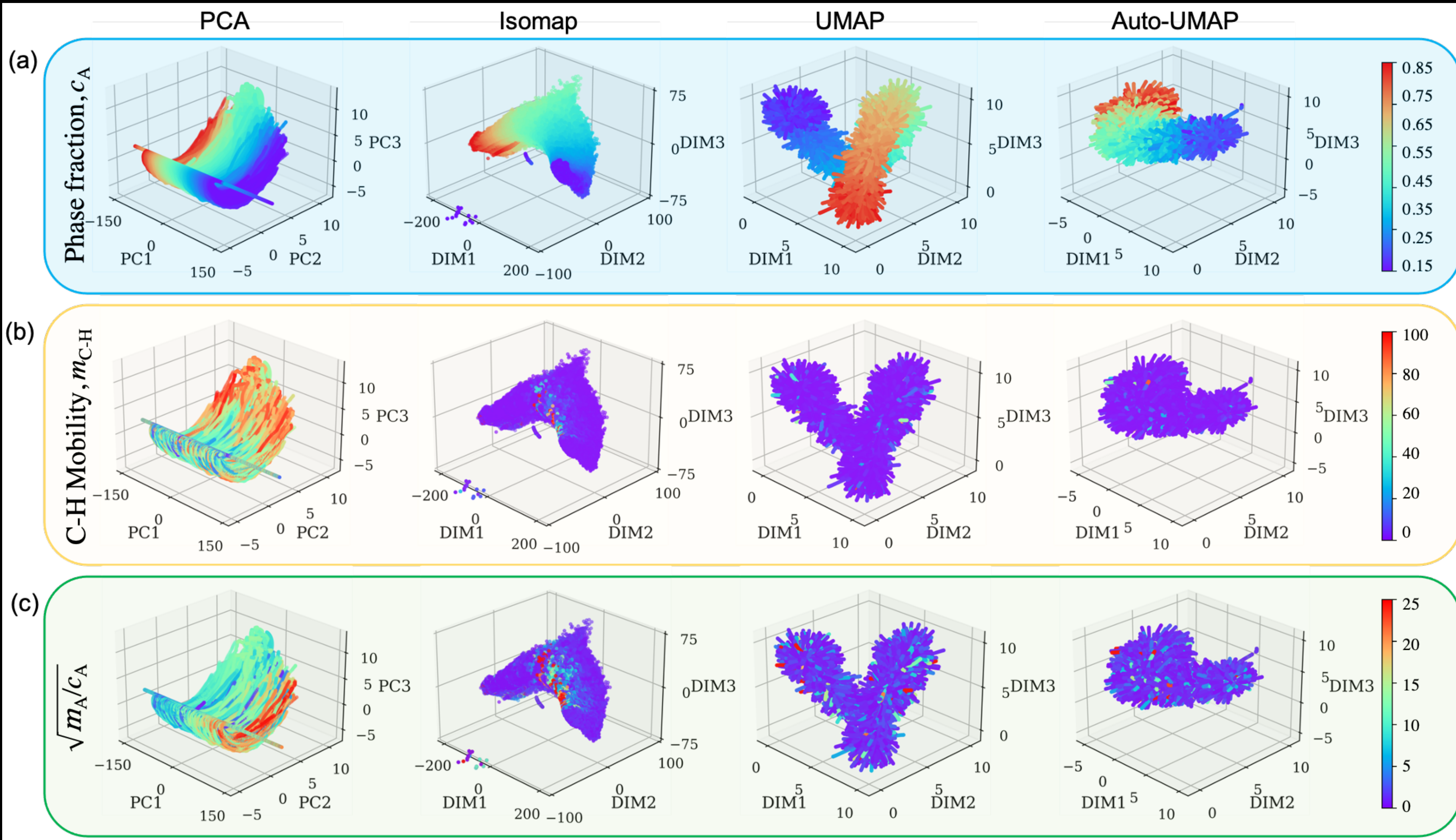


We Need Efficient Ways to: (i) Represent the Microstructure Evolution in Reduced Space and (ii) Learn the Time Evolution Via History-Dependent Algorithms

High-fidelity phase field | Dimension reduction | History-dependent ML | Accelerated phase field

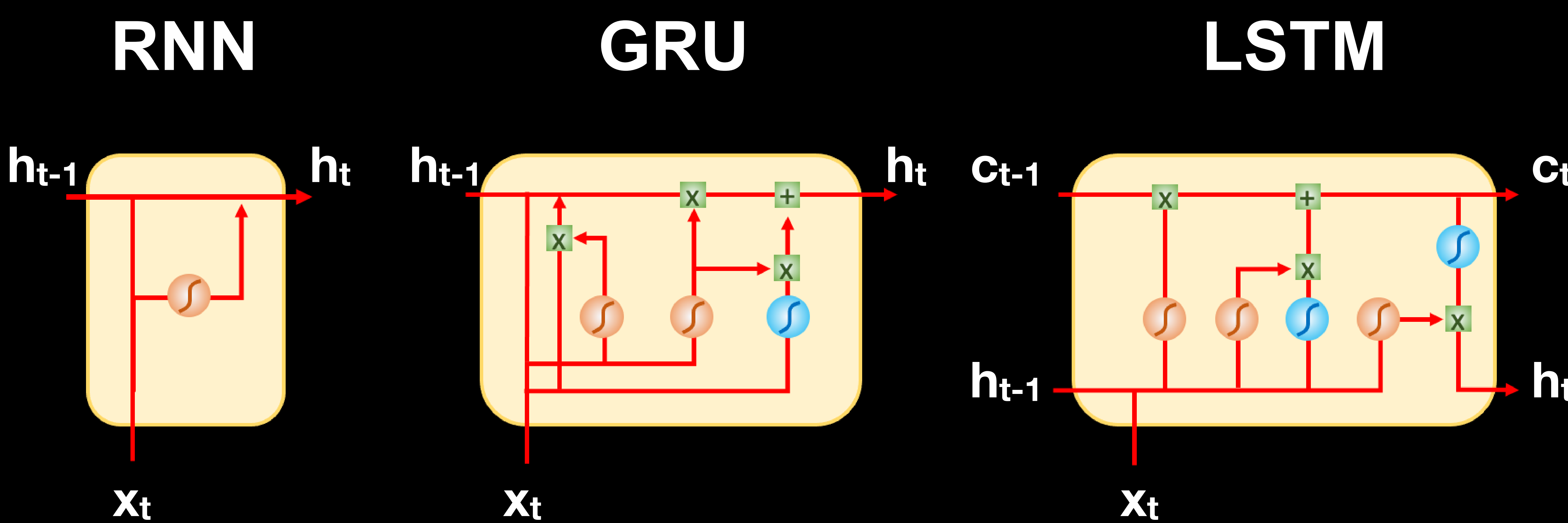


Linear vs. Non-Linear Embedding: Representation in Latent Space Matters



Time Forecasting: Our Problem Reduces to Learning the Microstructure Evolution in the Latent Space

Recurrent Neural Network (RNN): Flavors and Complexities



x: current state; h: history; c: copy

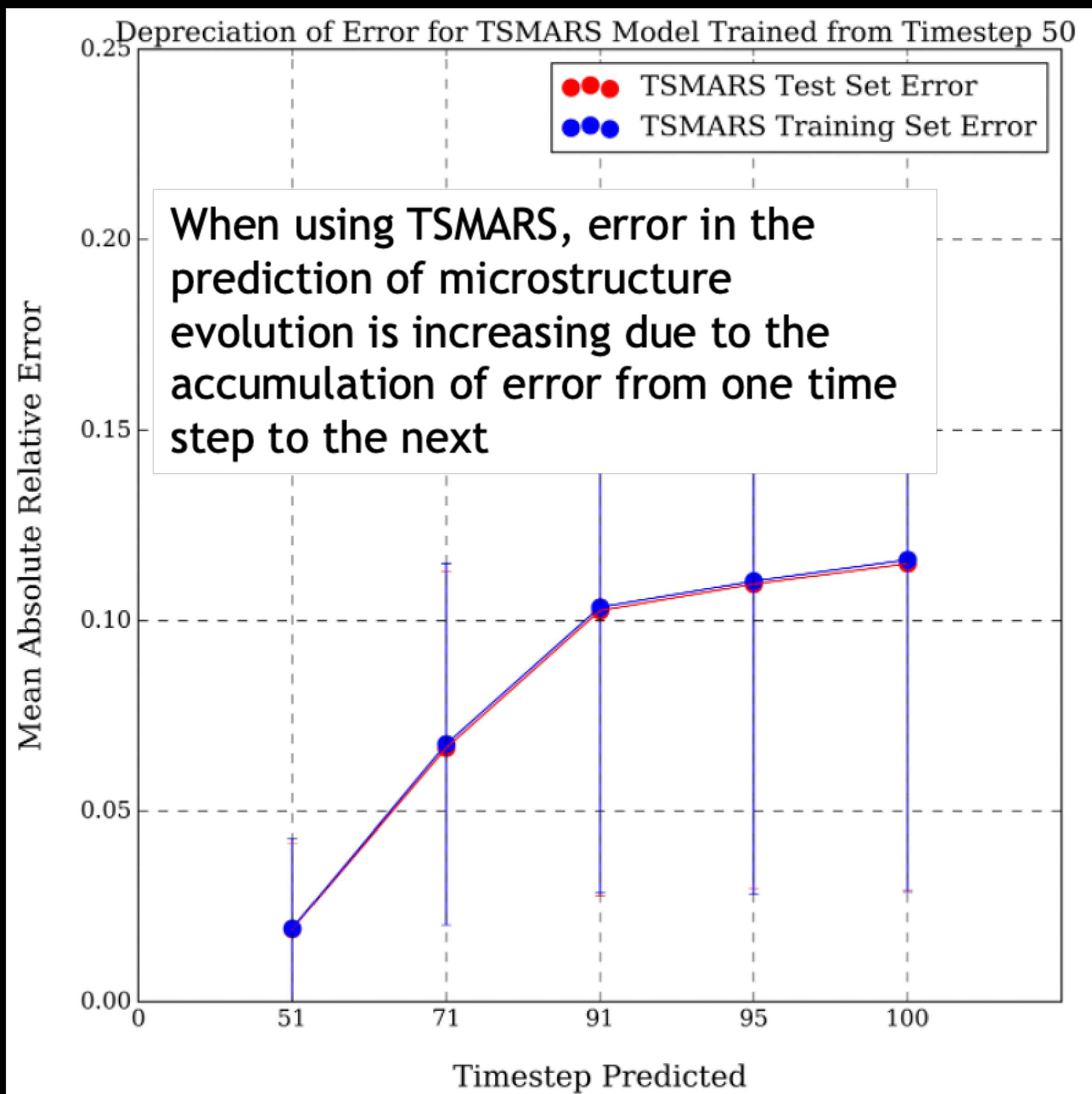
- Simple RNNs have no choice but to eventually forget due to vanishing gradient

- Two gates for GRU
- Output is h(t), depends on h(t-1) and x(t)

- Three gates for LSTM
- Output is h(t), depends on h(t-1), c(t-1), and x(t)

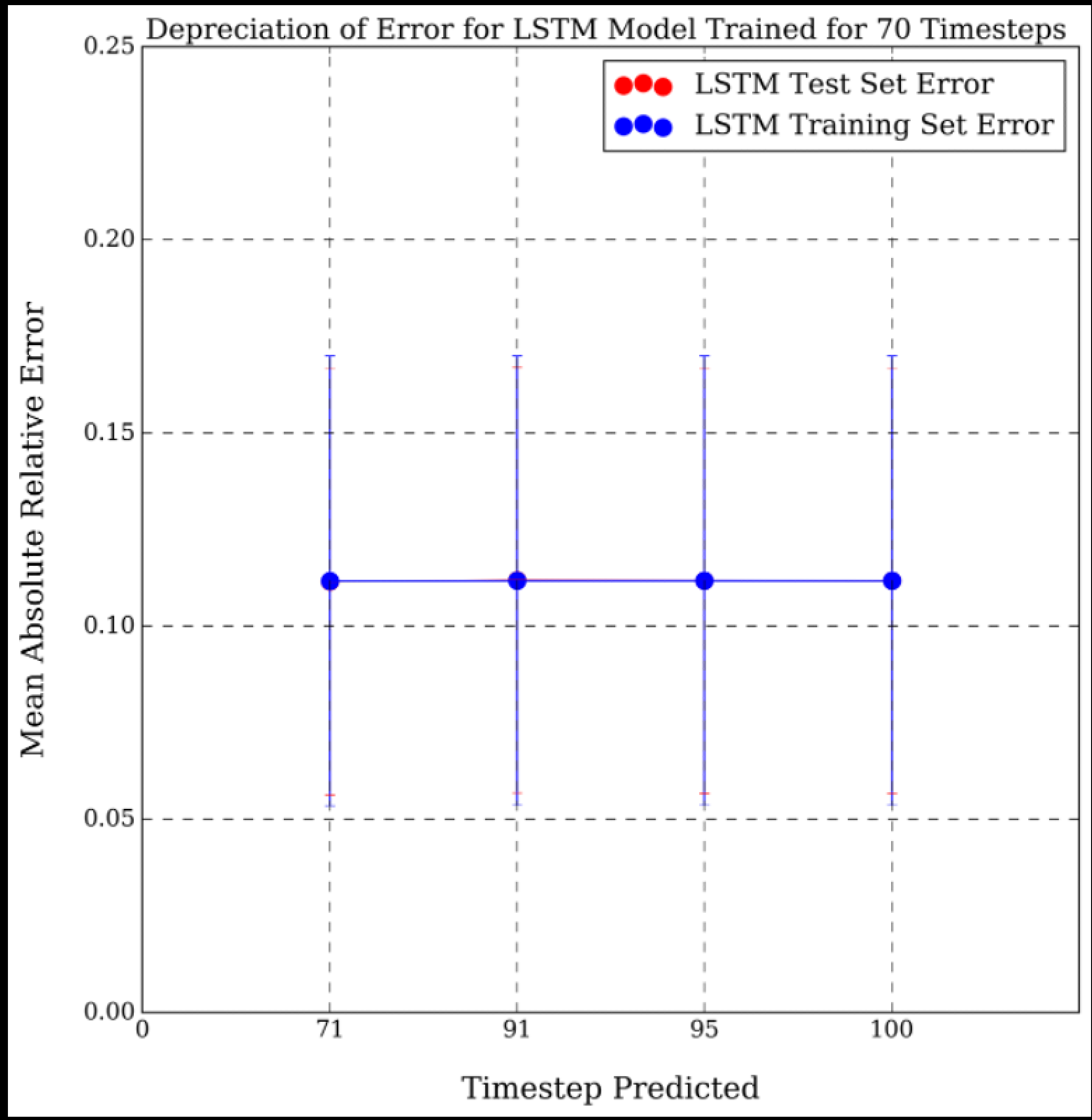
Why Do We Need a RNN Strategy?

TSMARS



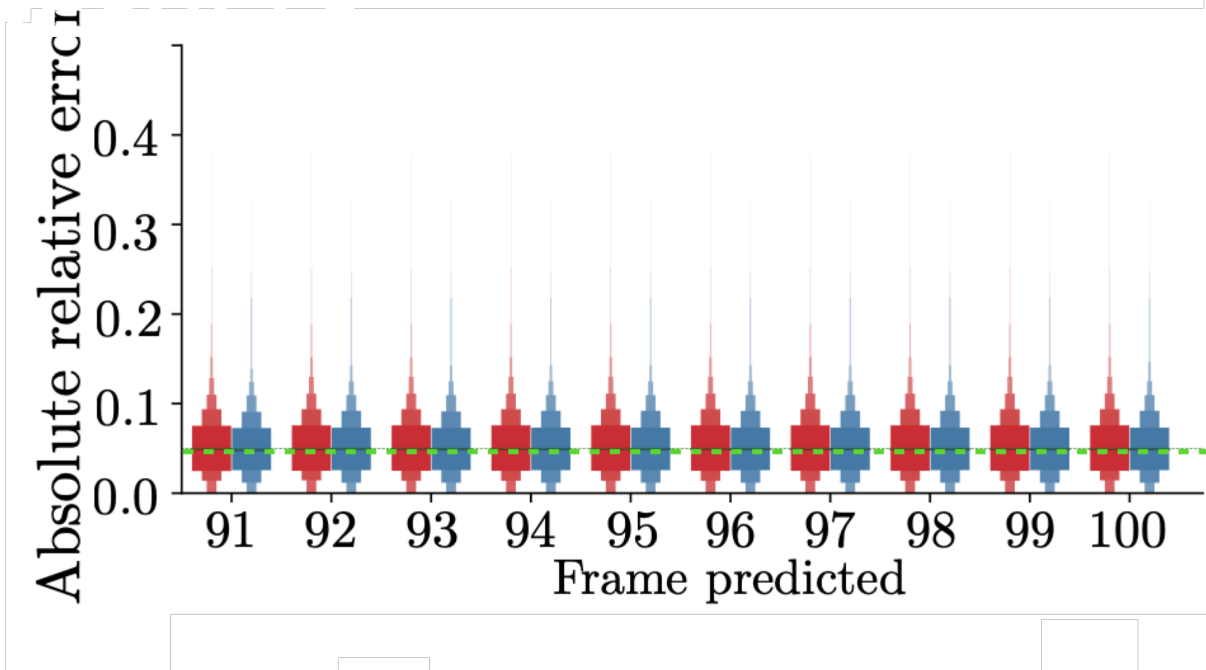
Good for data augmentation

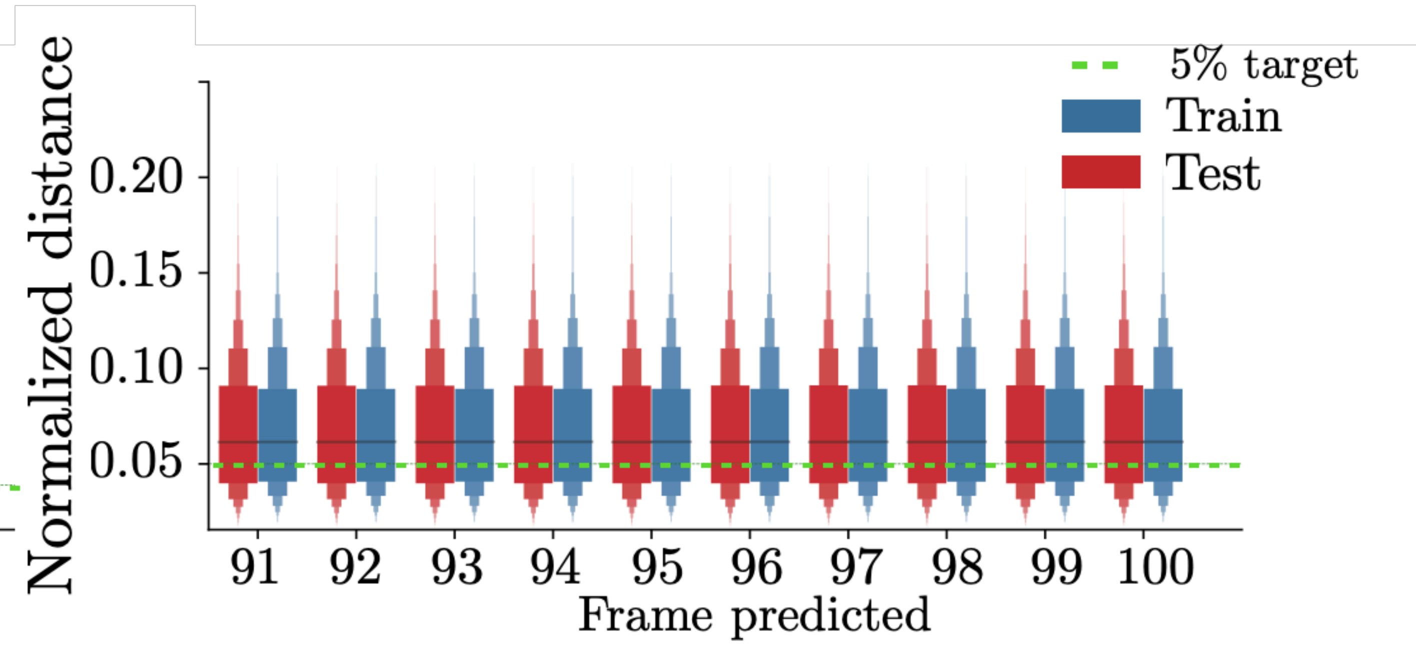
RNN

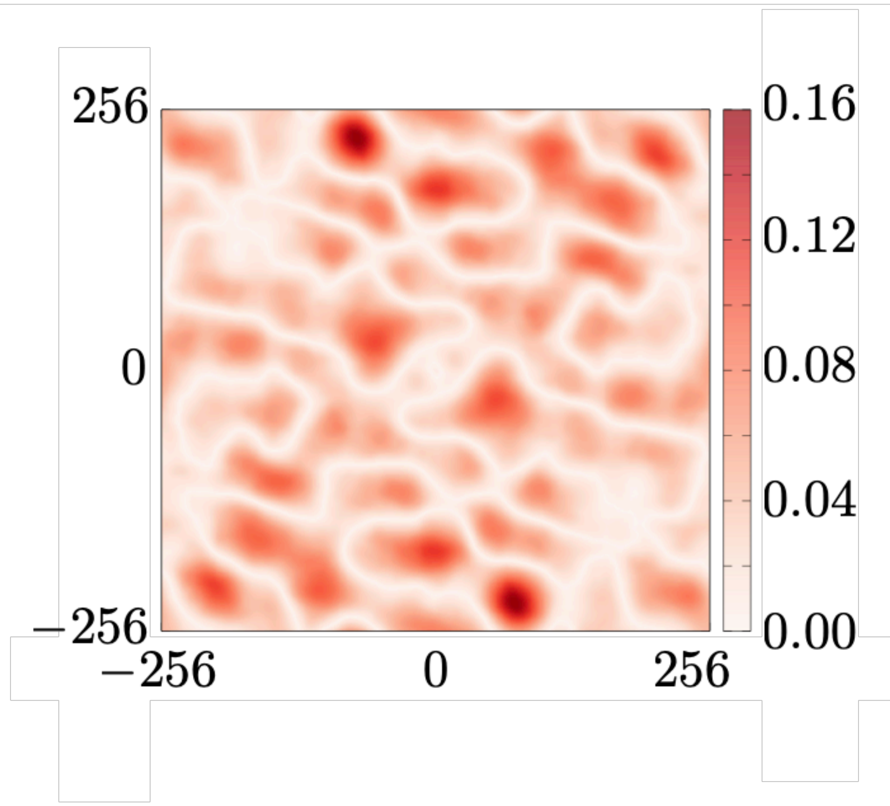


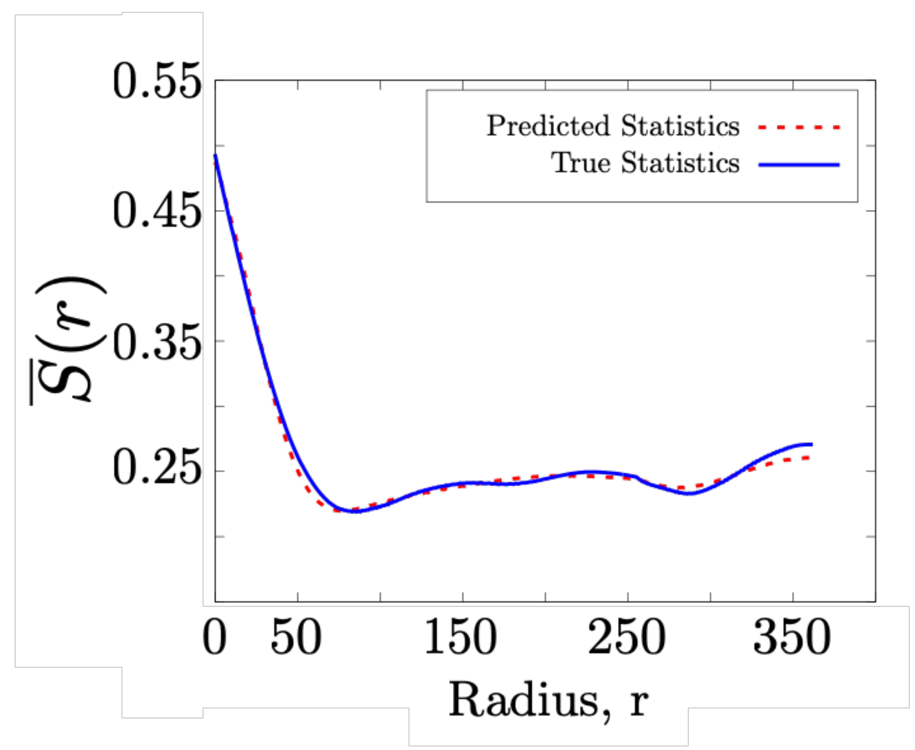
Good for extrapolation

We Can Achieve Similar Accuracy with our RNN/GRU/LSTM-Trained Models As Compared to High-fidelity Phase-Field

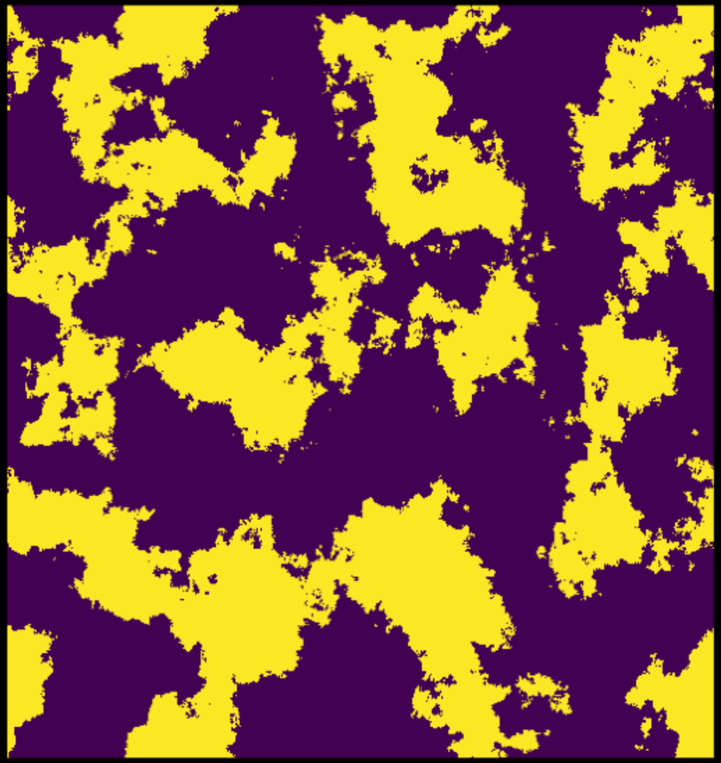


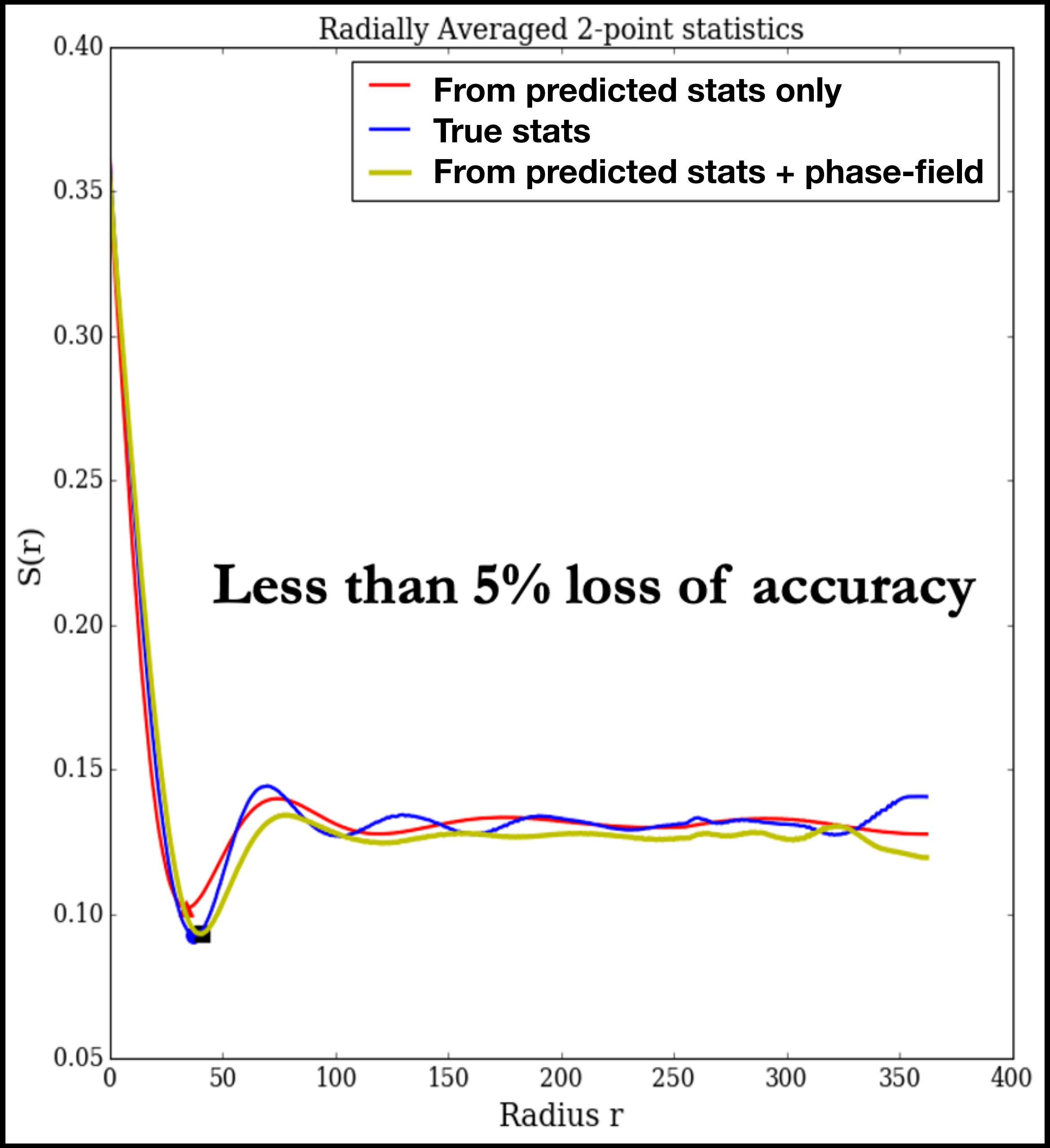






Feeding Back our Predictions Into PF Provides an Efficient way to Smooth-out the Reconstructed Microstructure and Course-Correct the Physics


LSTM only



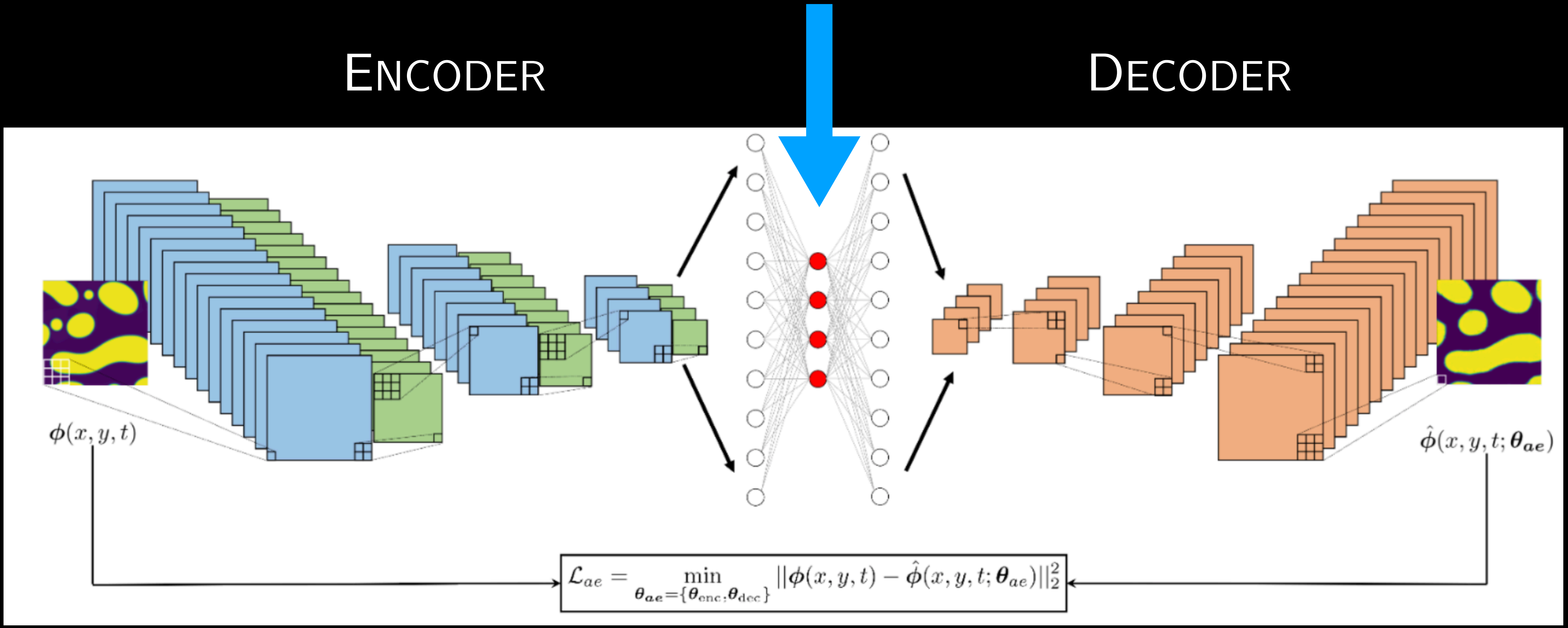

LSTM + phase field

Bypassing Statistical Description of Microstructure: Encode and Decode…

Time series in Latent Space

Encoder

Decoder



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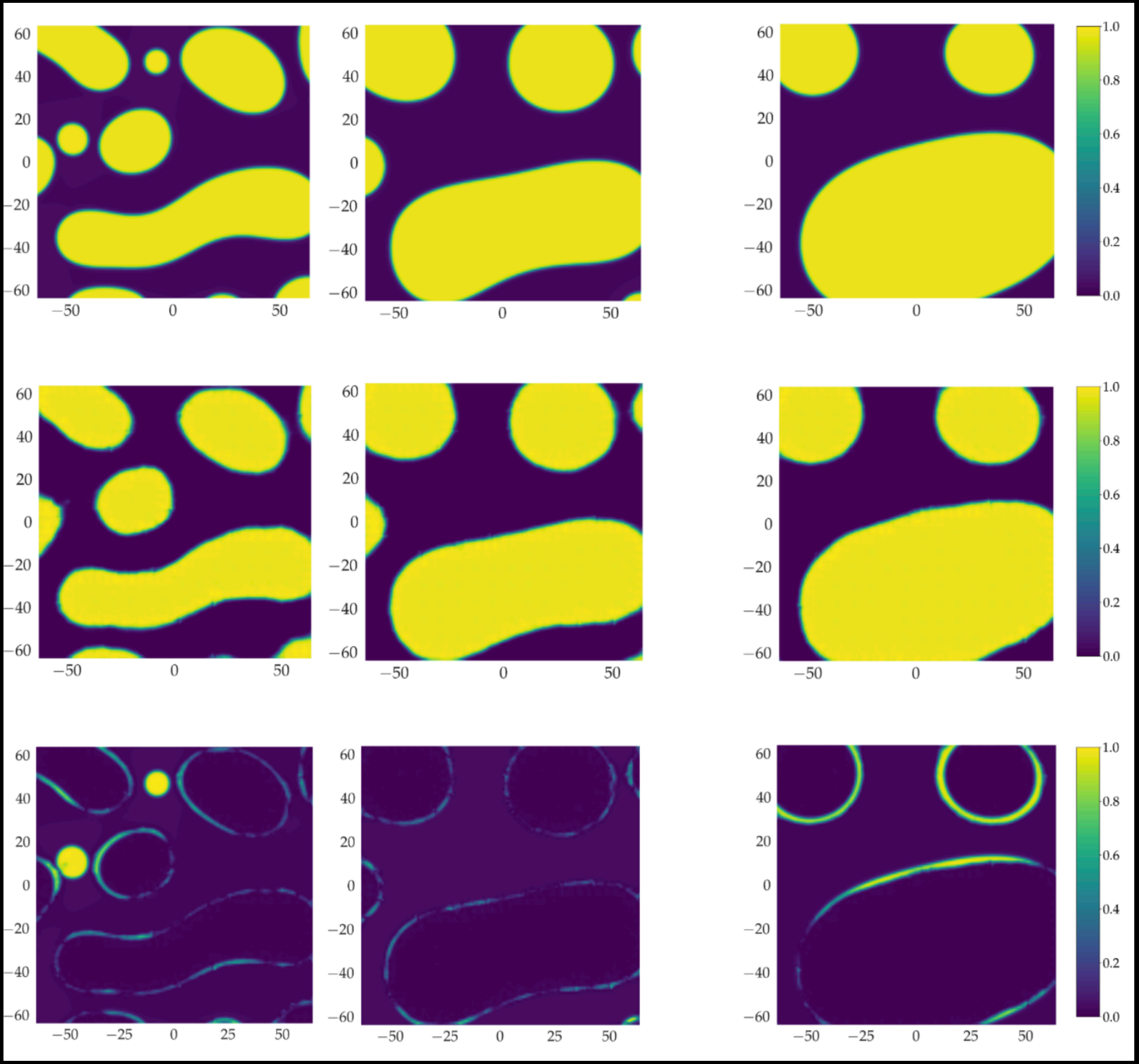

Towards Agility Of Microstructure Performance Assessment

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50000 sims?

9 years

with high-fidelity PF

25-50 mins

with accelerated PF

45,000 faster

Concluding Remarks: This is What Happens When a Material Scientist Tries to Use ML Methods

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  - **Challenge:** Capturing multiple length scales, short vs. long range interactions

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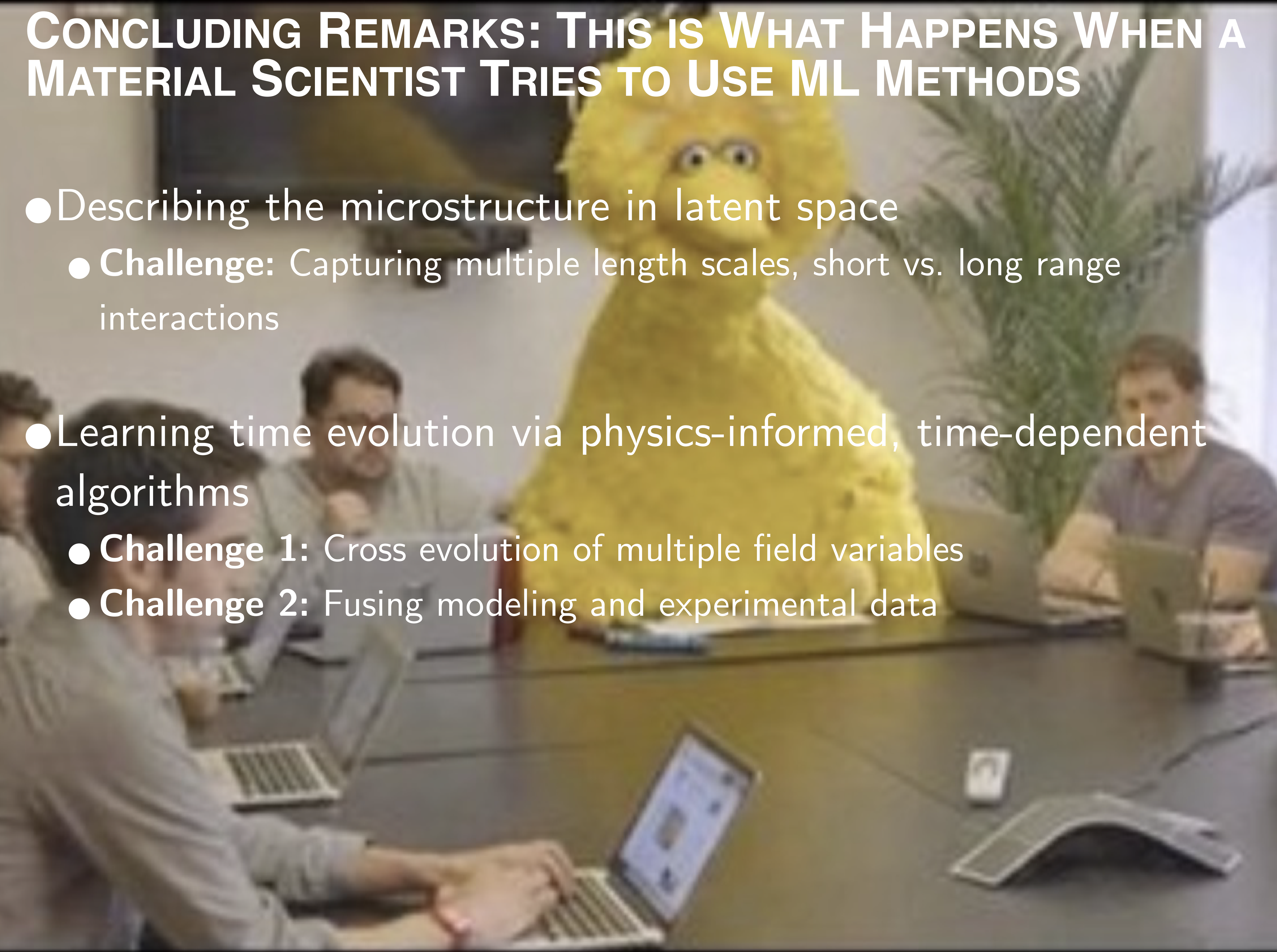
  - **Challenge:** Capturing multiple length scales, short vs. long range interactions
- Learning time evolution via physics-informed, time-dependent algorithms
  - **Challenge 1:** Cross evolution of multiple field variables
  - **Challenge 2:** Fusing modeling and experimental data



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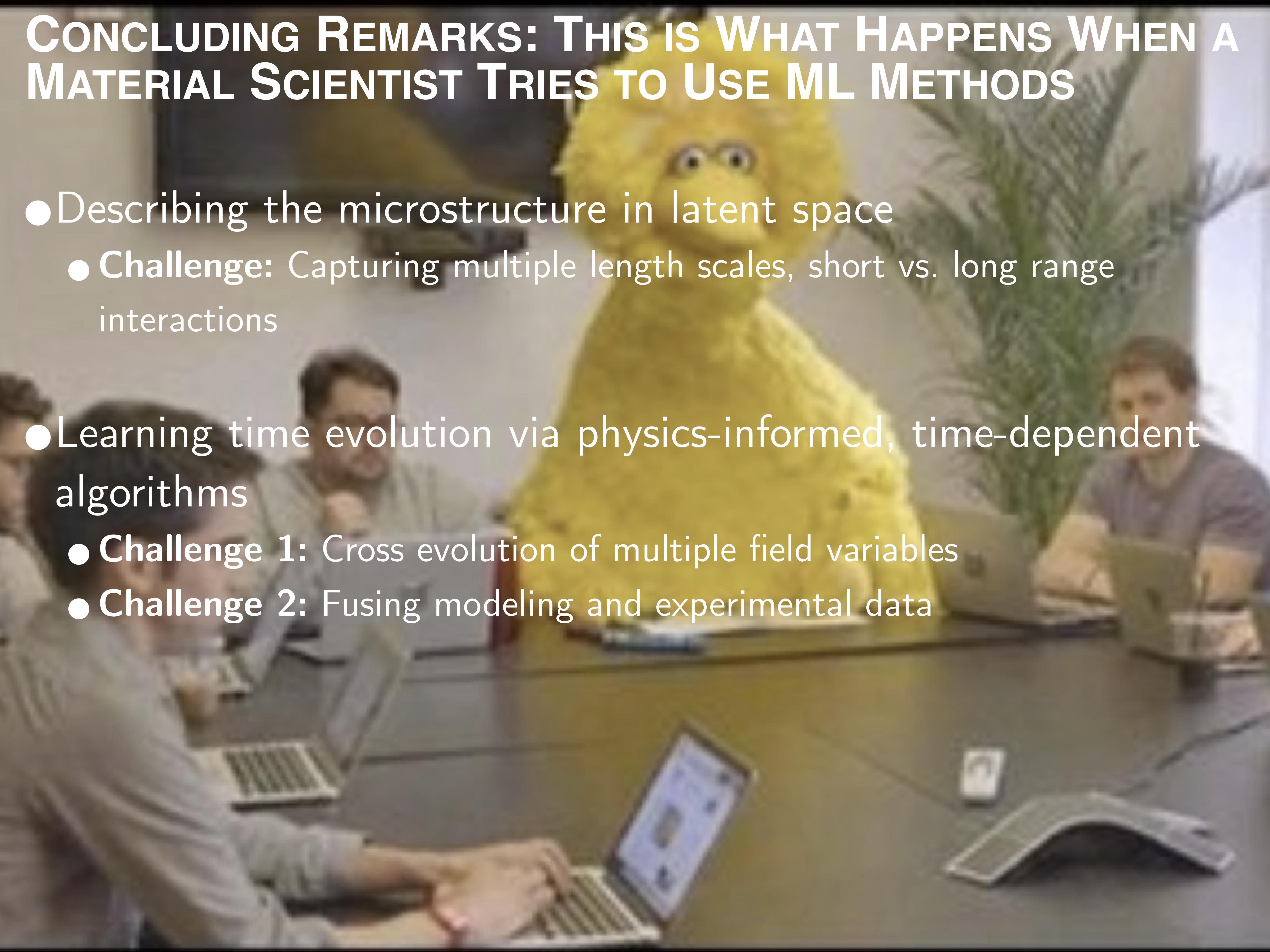

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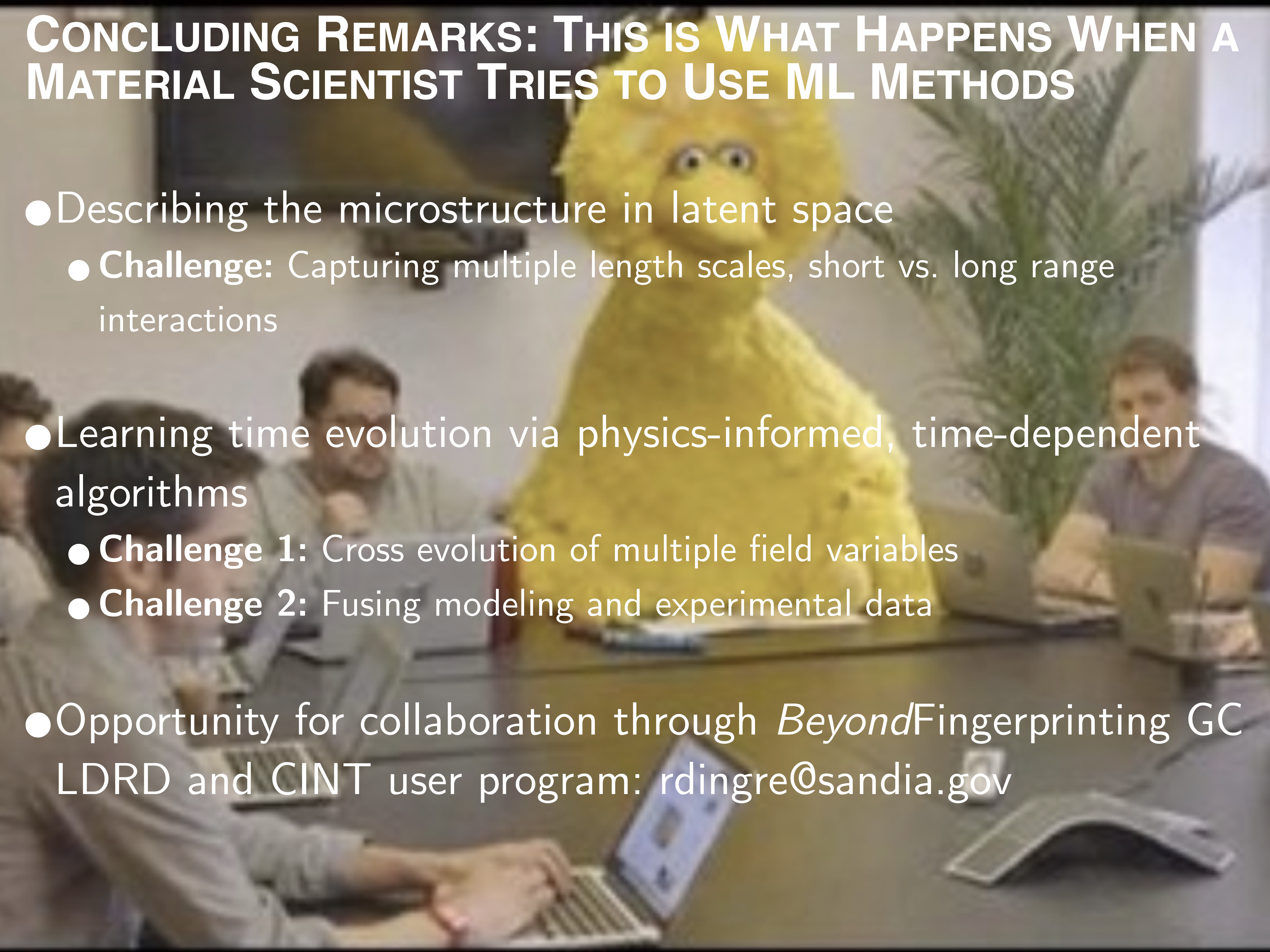

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  - **Challenge 2:** Fusing modeling and experimental data
- Opportunity for collaboration through *Beyond*Fingerprinting GC LDRD and CINT user program: rdingre@sandia.gov

BIG SCIENCE AT THE NANOSCALE

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- Soft, Biological, and Composite Nanomaterials

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