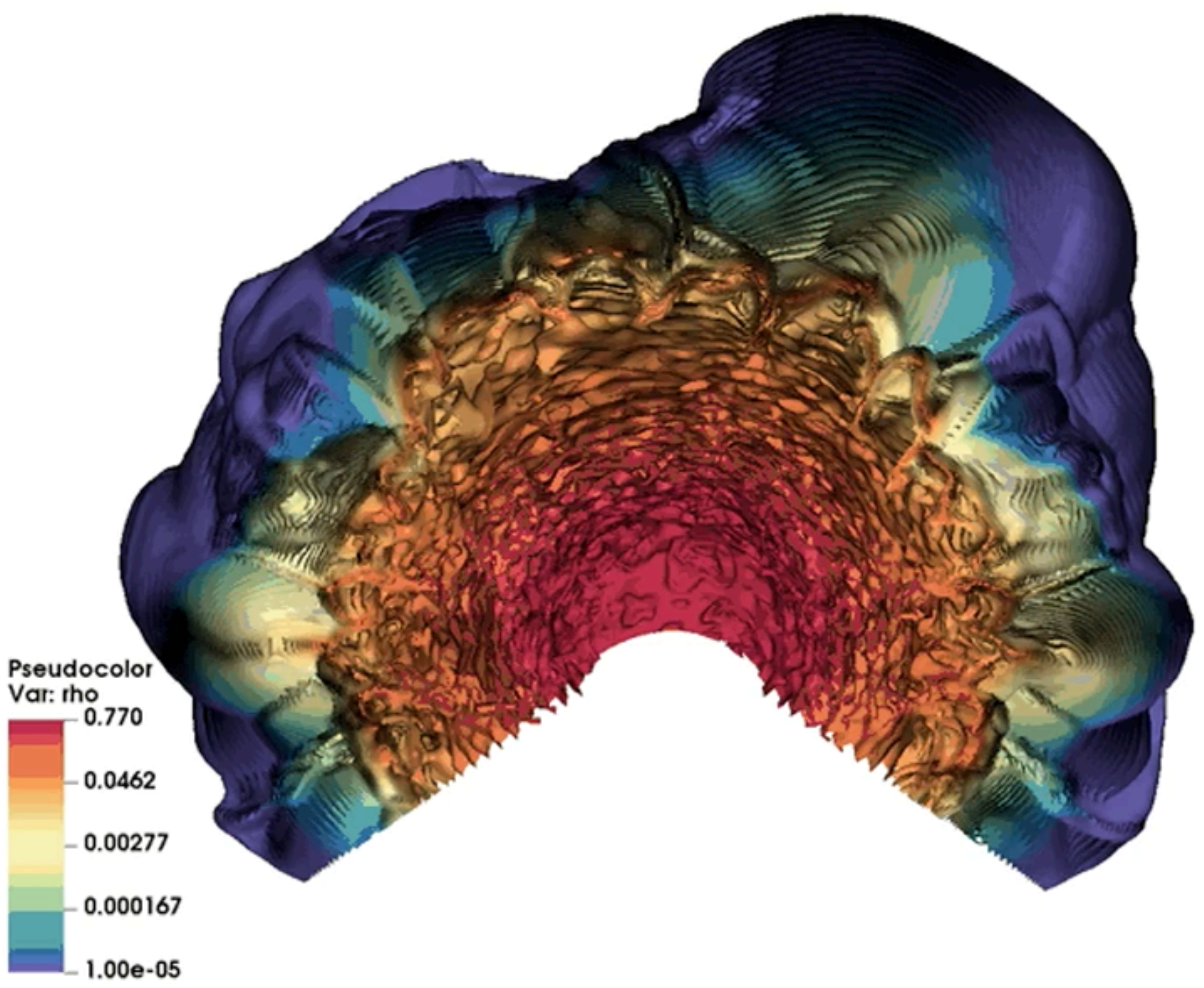
Multiple Physics Pretraining for Spatiotemporal Surrogate Models

Project led by Michael McCabe, Bruno Regaldo, Liam Parker, Ruben Ohana, Miles Cranmer

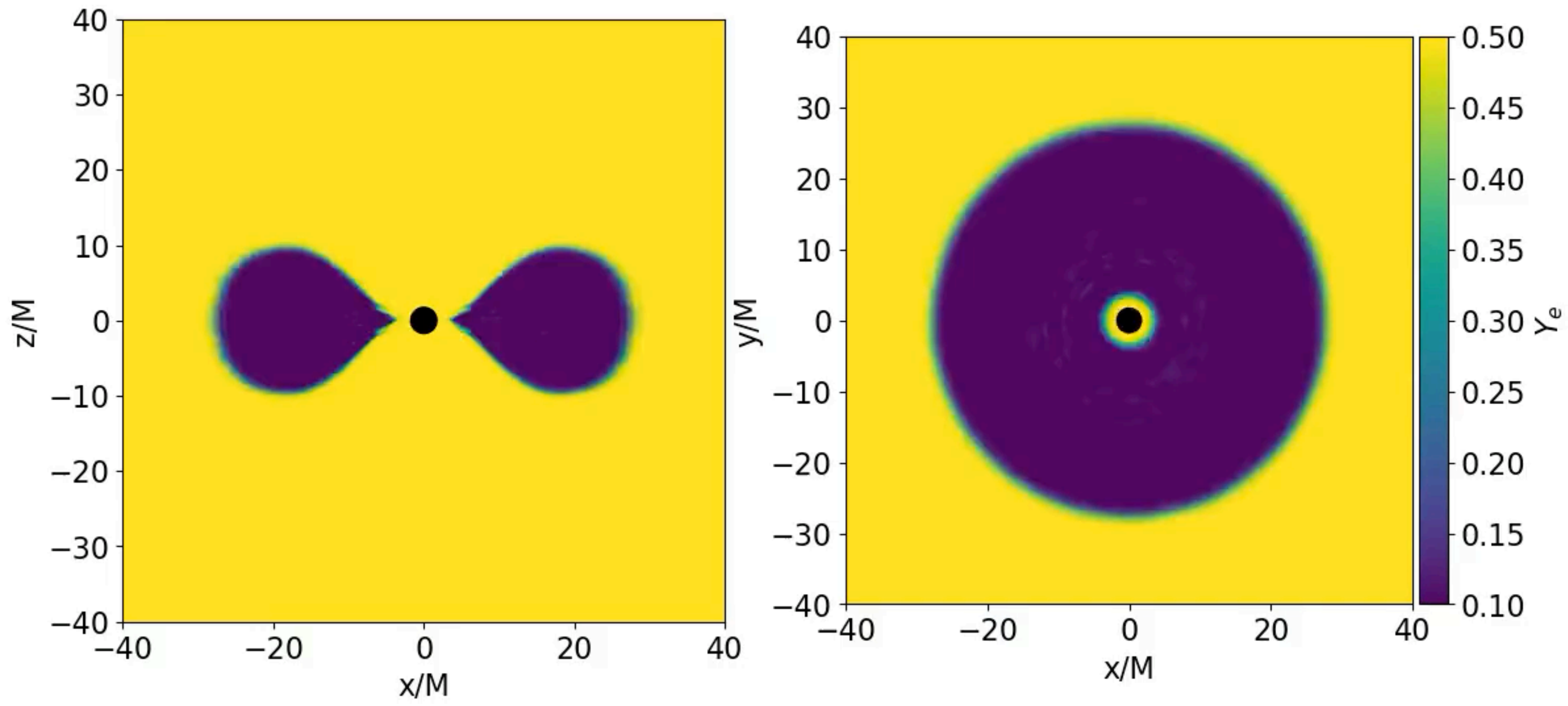
Polymathic

Where is machine learning useful for simulation?

Accelerating Simulation



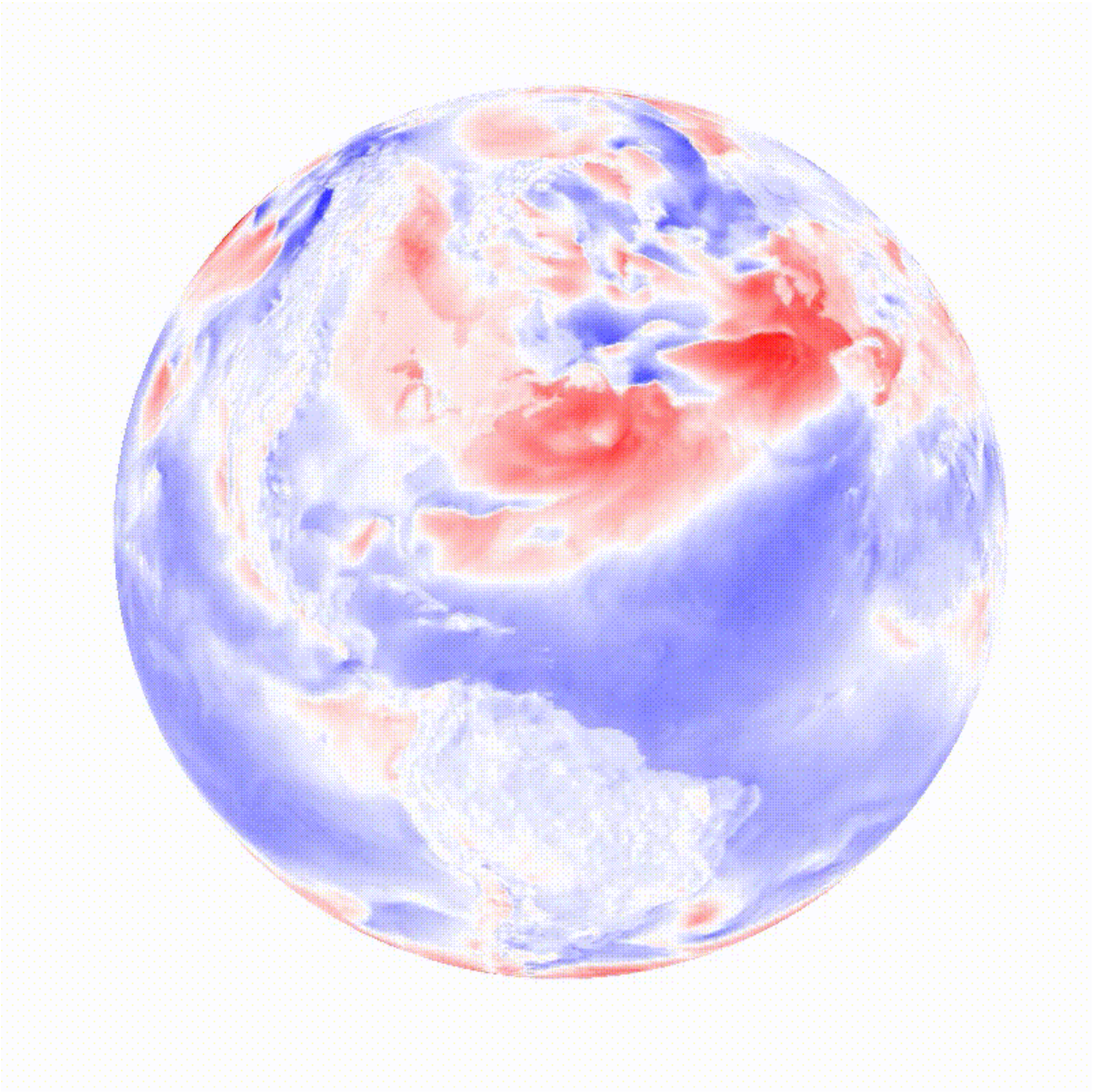
Goldberg, Jiang & Bildsten. 2021.



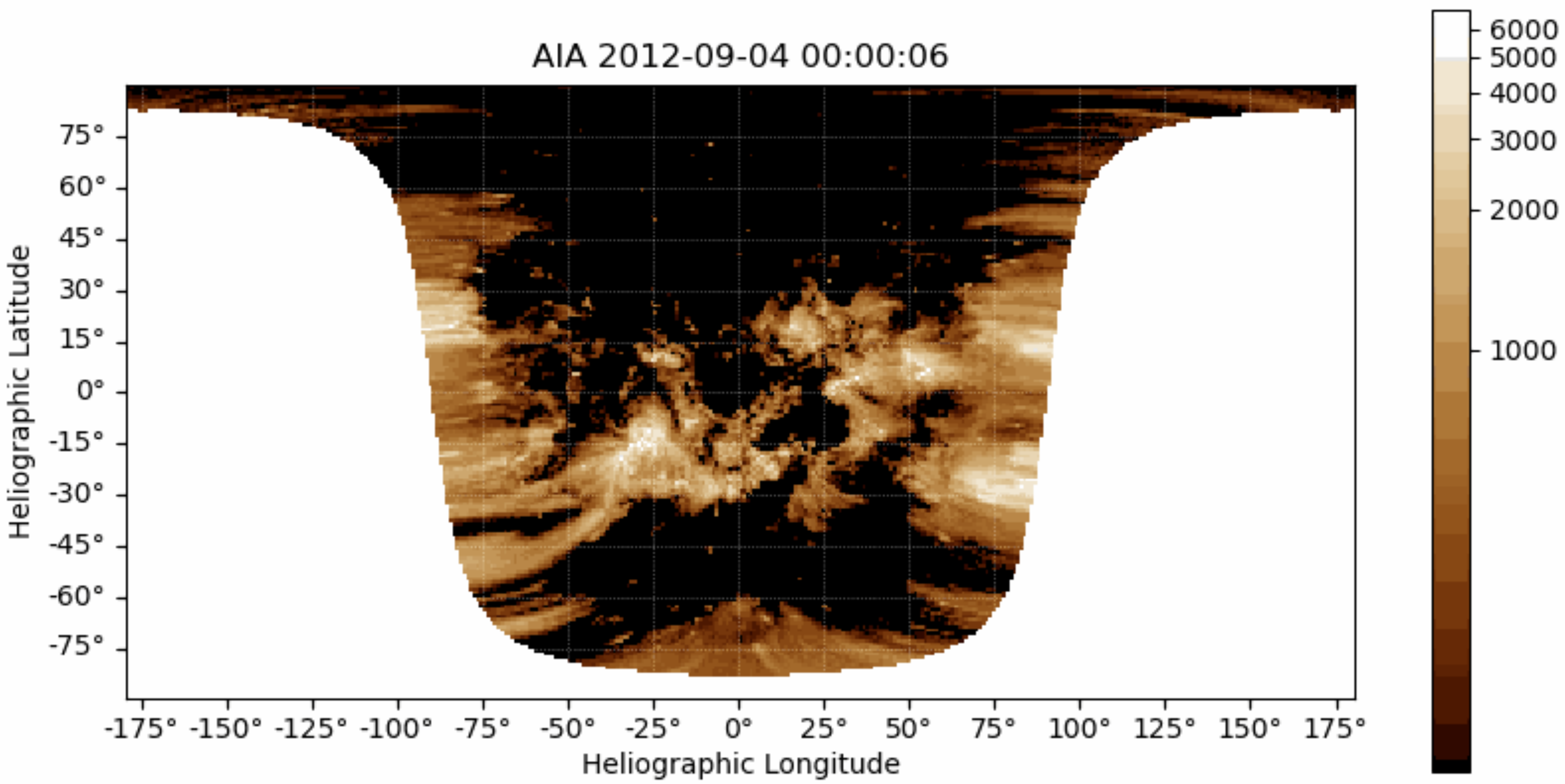
Miller et al., 2019.

Where is machine learning useful for simulation?

Poorly Specified or Imperfectly Observed Dynamics



The Earth



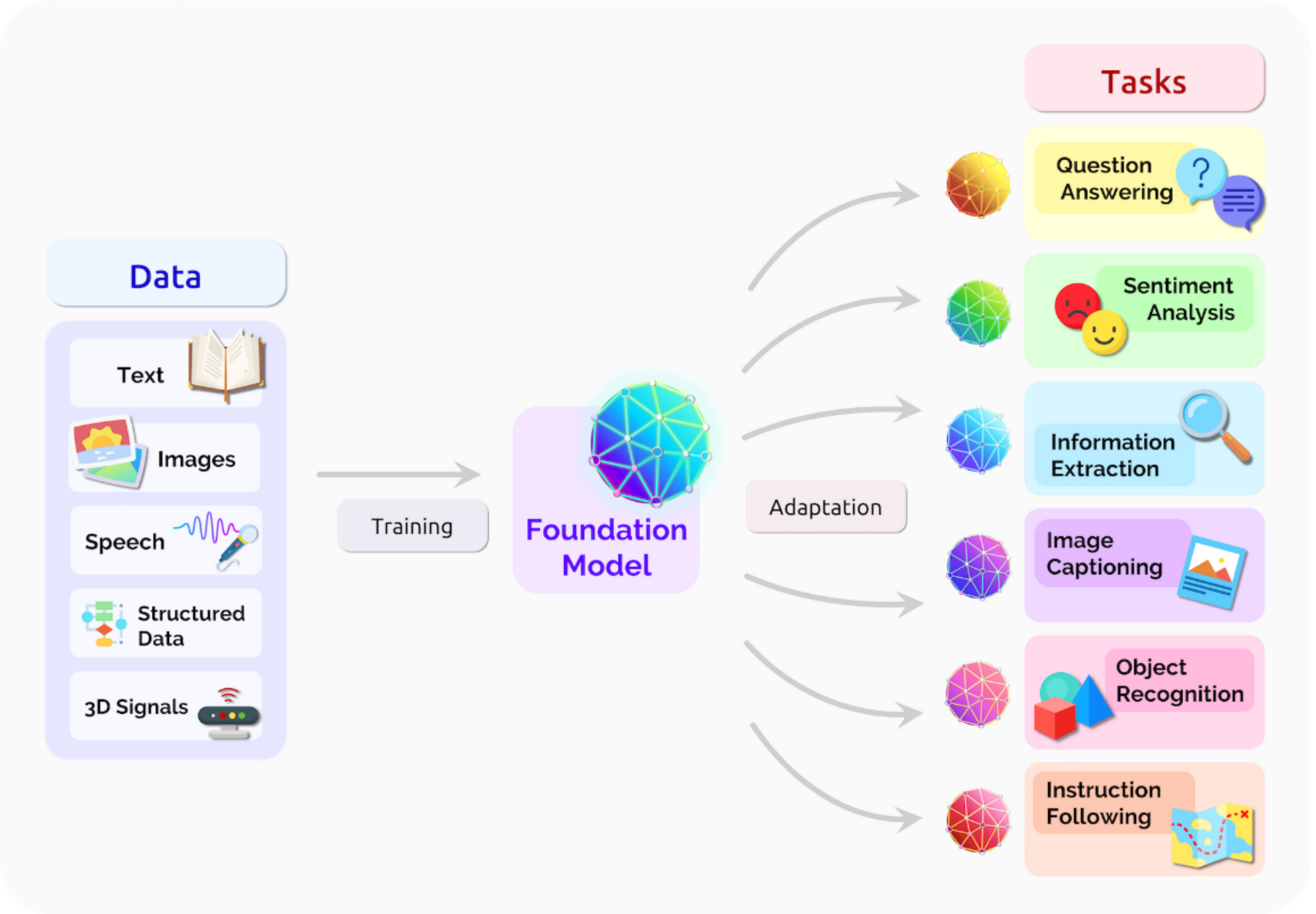
The Sun

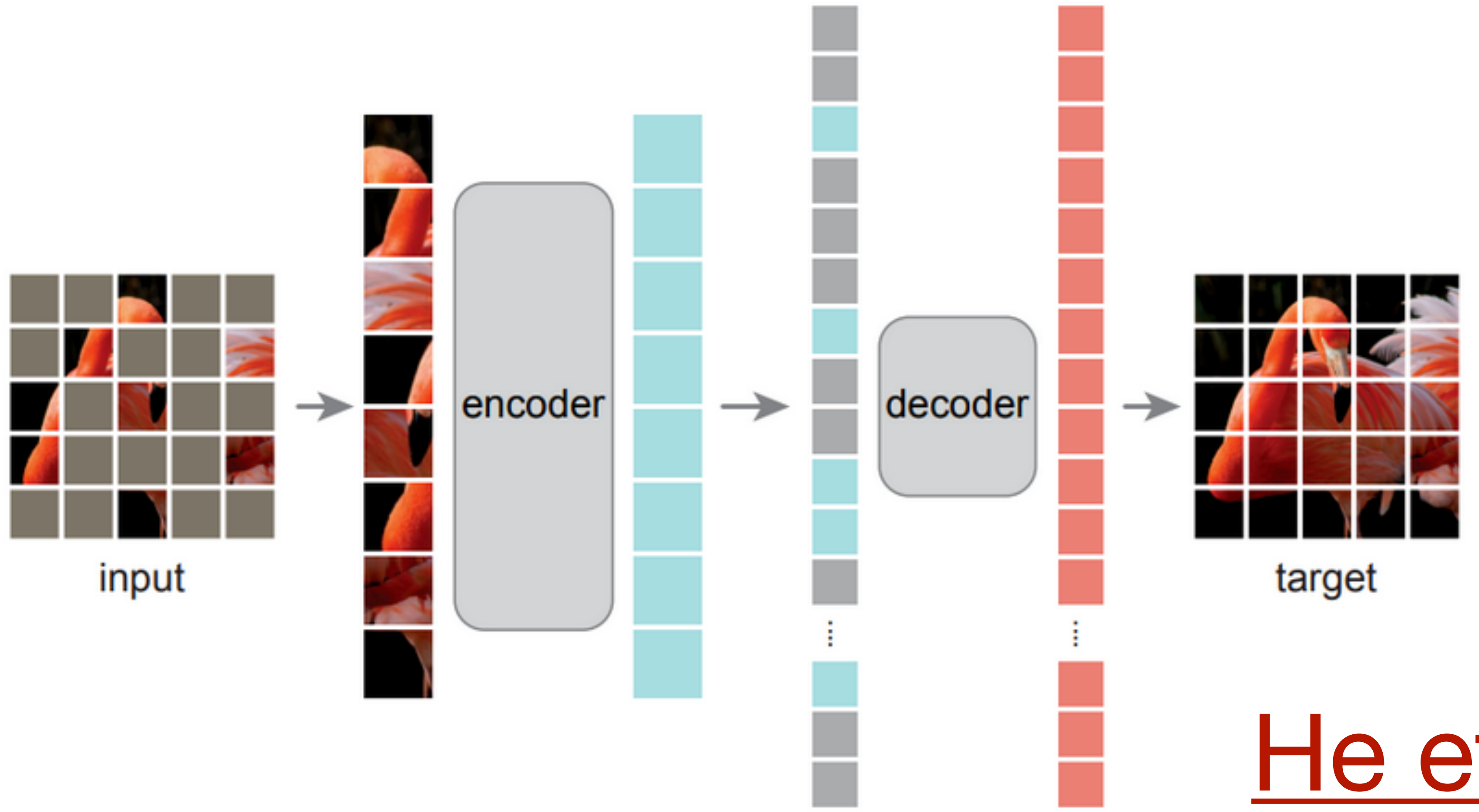
Both are settings where data will be inherently limited*

*Weather is an exception here

The Rise of the Foundation Model Paradigm

- **Foundation Model approach**
  - **Pretrain** models on objectives that do not require manual labeling to get access to very large datasets.
  - **Adapt** pretrained models to downstream tasks.





He et al. 2021

Bommansani et al. 2021

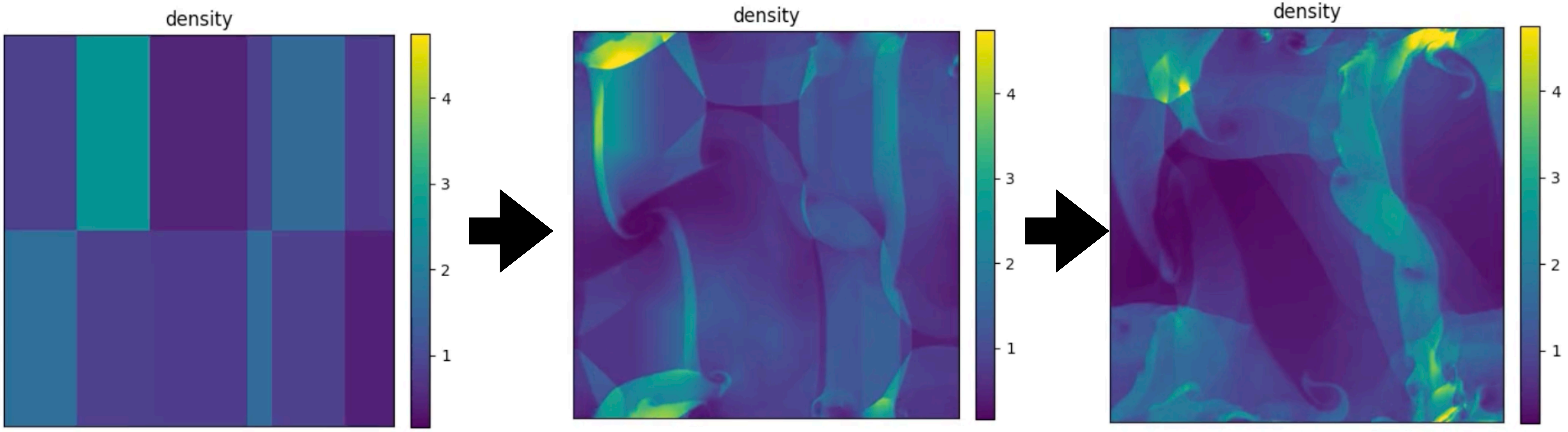
“Transferring” this approach to physical simulation

Key Questions

1. Does pretraining on **partially overlapping physics** help few-shot adaptation to new systems?
2. Is it possible to learn from sufficiently diverse physics to **maximize our attack surface** for transfer?

What do we mean by physics in this case?

Dynamics - The ability to estimate the evolution of a system given initial conditions



T=0 T=1 T=2

Simplified Example

Scalar Transport - Compositional Systems

Advection: $$\frac{\partial \psi}{\partial t} + \nabla \cdot (v\psi) = 0$$

Diffusion: $$\frac{\partial \psi}{\partial t} + \nabla \cdot (-\delta \nabla \psi) = 0$$

Advection-Diffusion: $$\frac{\partial \psi}{\partial t} + \nabla \cdot (v\psi - \delta \nabla \psi) = 0.$$

Simplified Example

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1. Train on large amounts (100k) of advection and diffusion simulations.

2. Finetune on restricted advection-diffusion data.

Simplified Example

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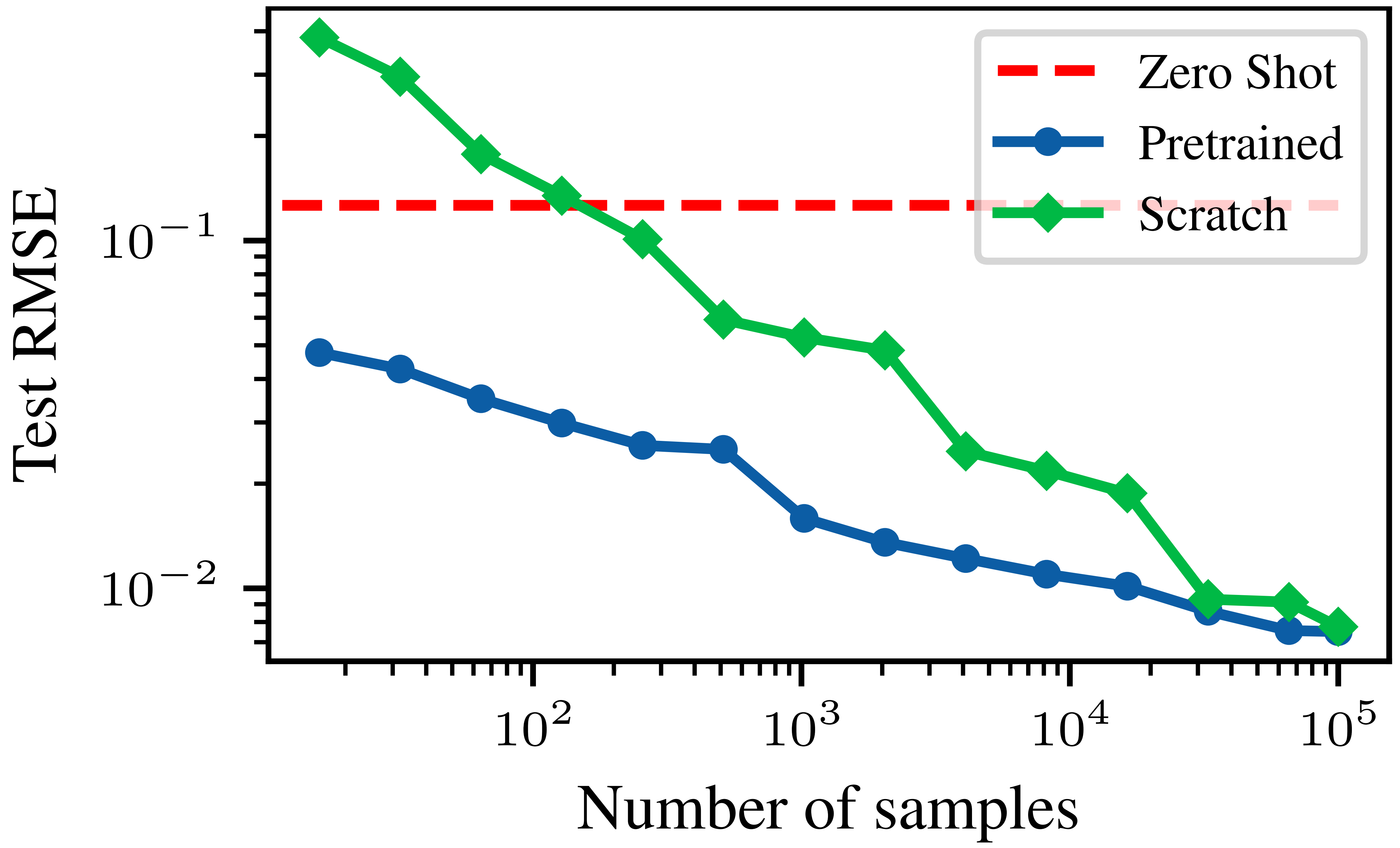

Simplified Example

Compositional Systems

But how can we do this for complex, nonlinear dynamics?

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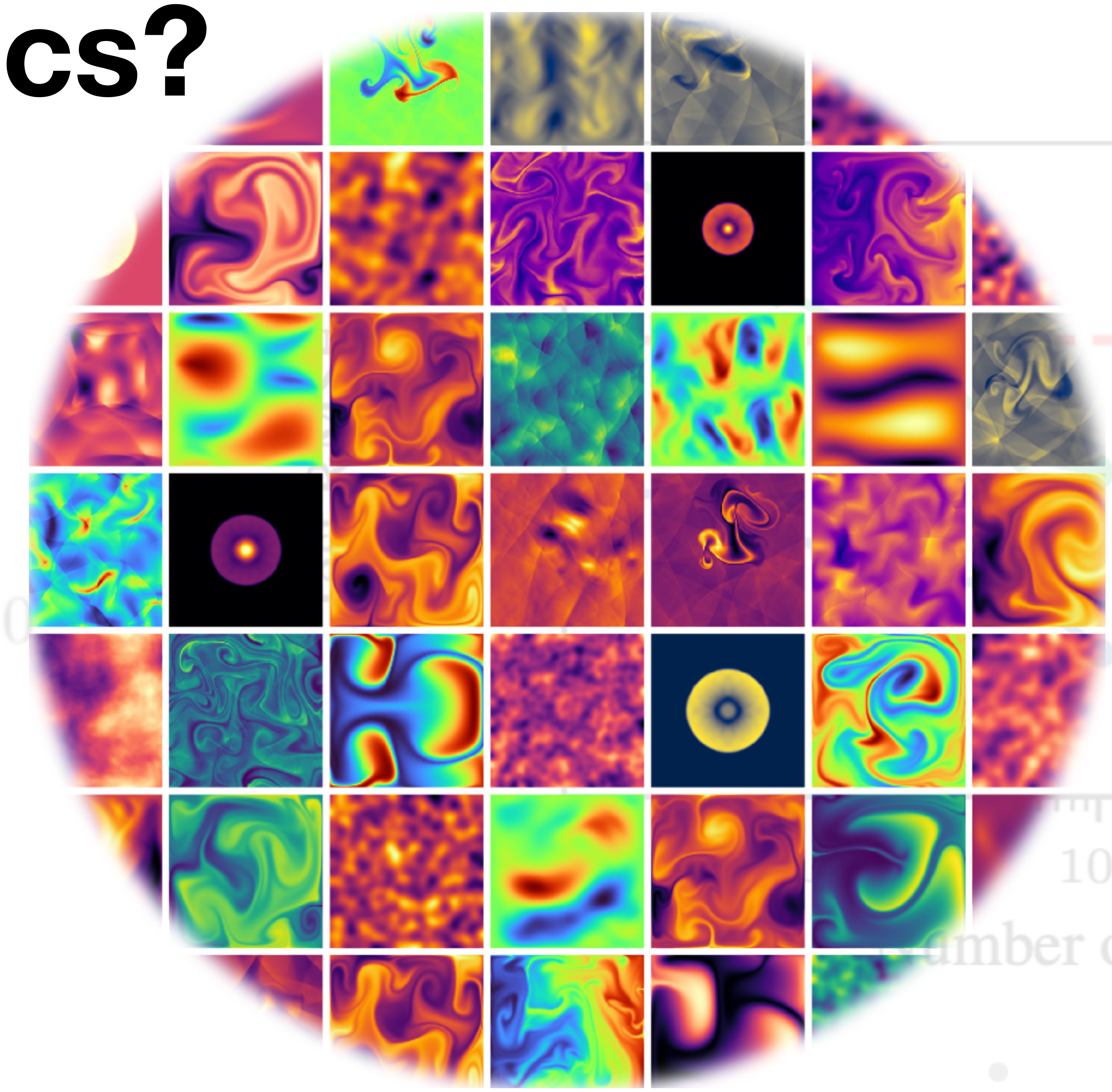
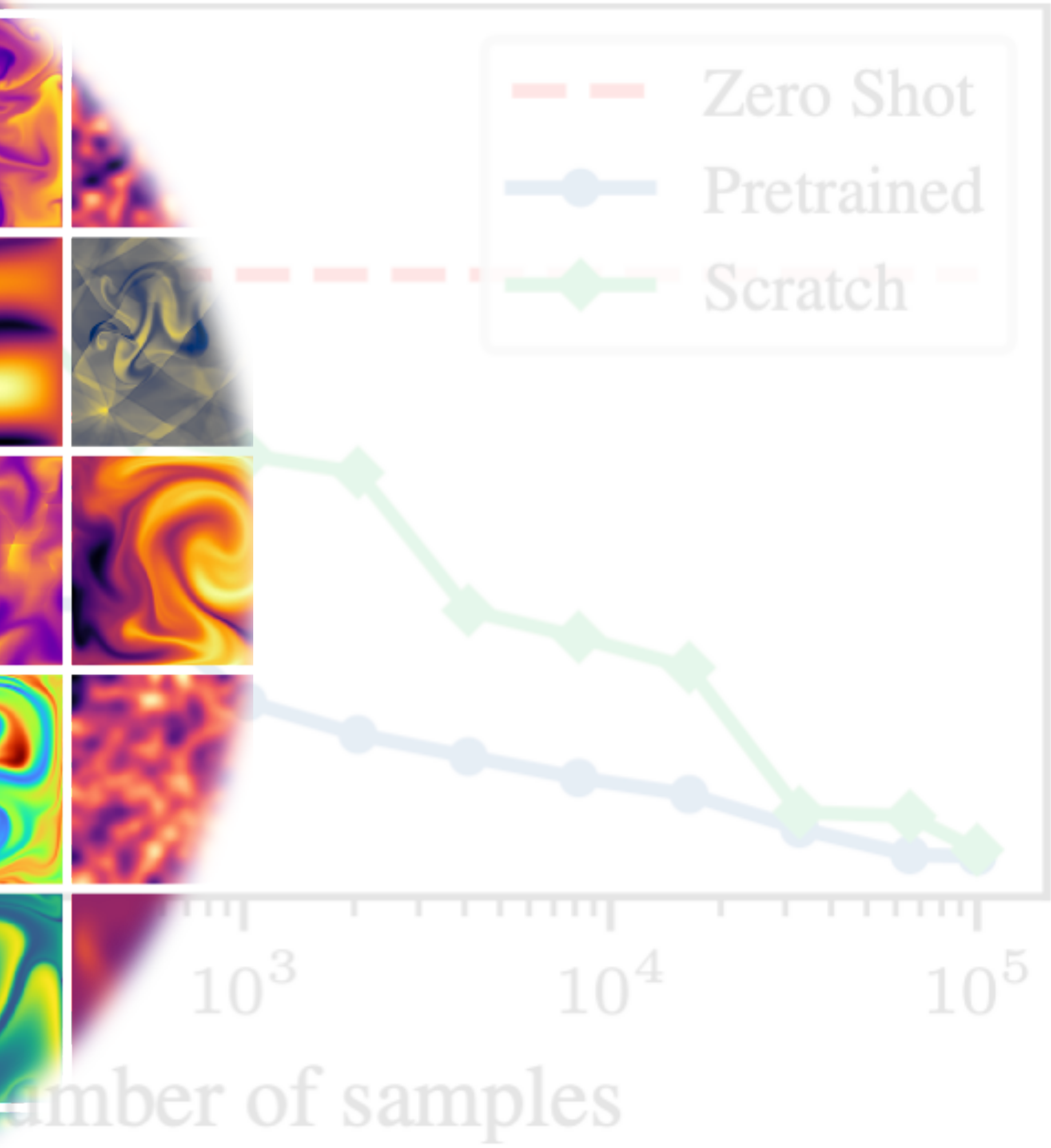




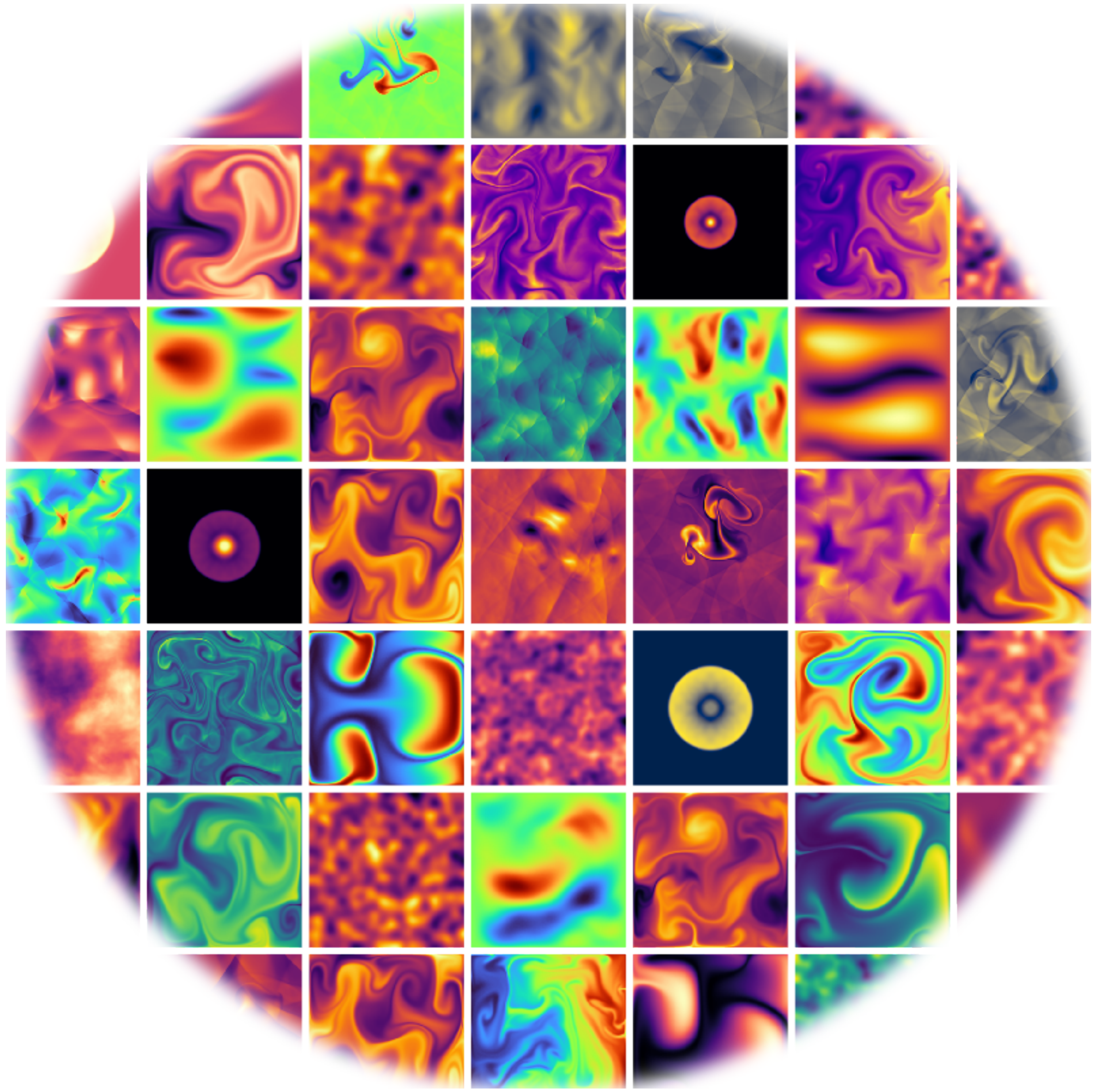
Training Data

PDEBench (Takamoto et al., 2022)

All 2D time-dependent problems:

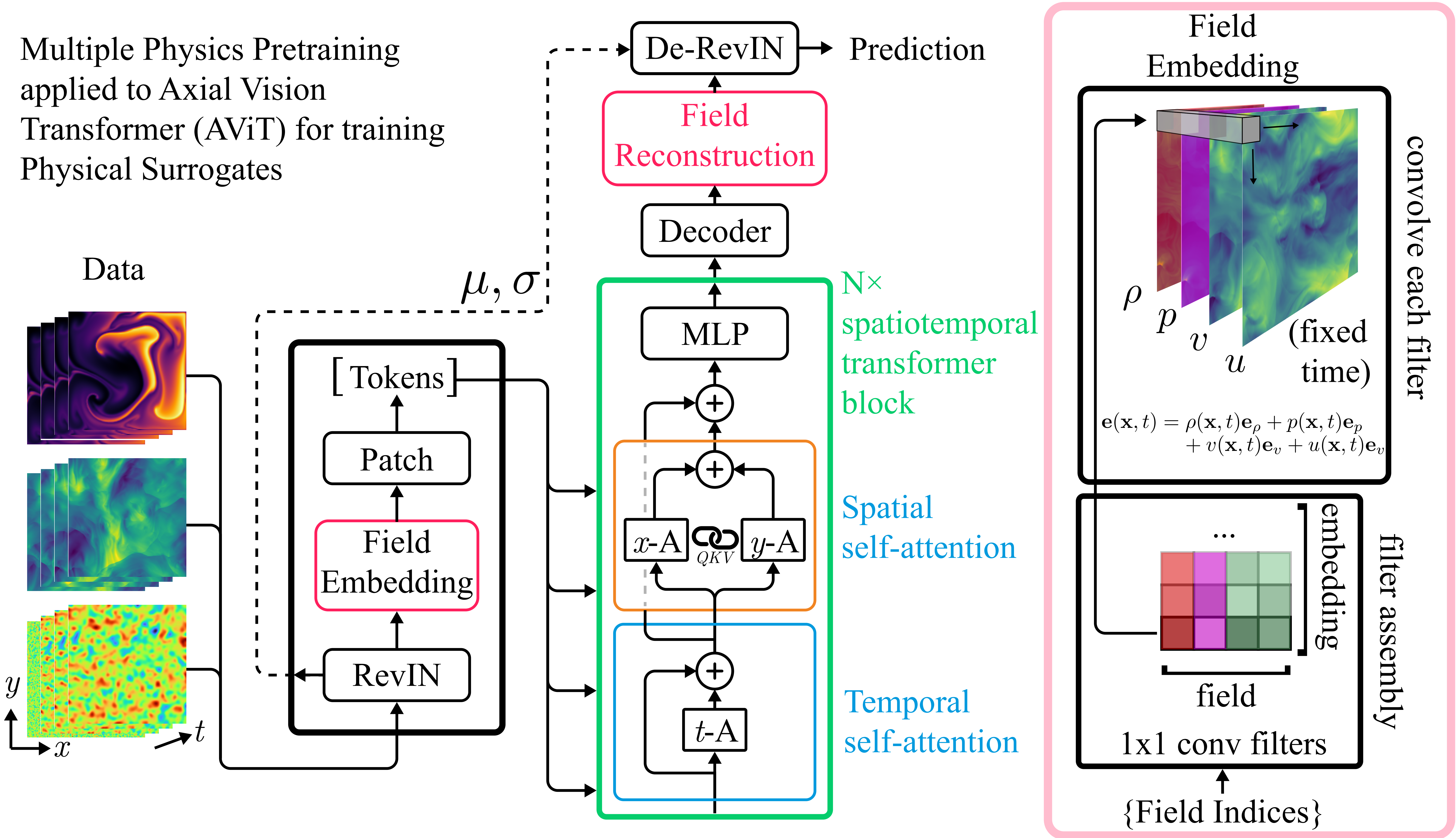
- 2D Diffusion-Reaction
  - BC - No flow
- Shallow Water Equations (Dam Break)
  - BC - Neuman
- Incompressible Navier-Stokes
  - BC - Dirichlet
- Compressible Navier Stokes
  - BC - Periodic

Sampled at variety of ICs and system parameters.



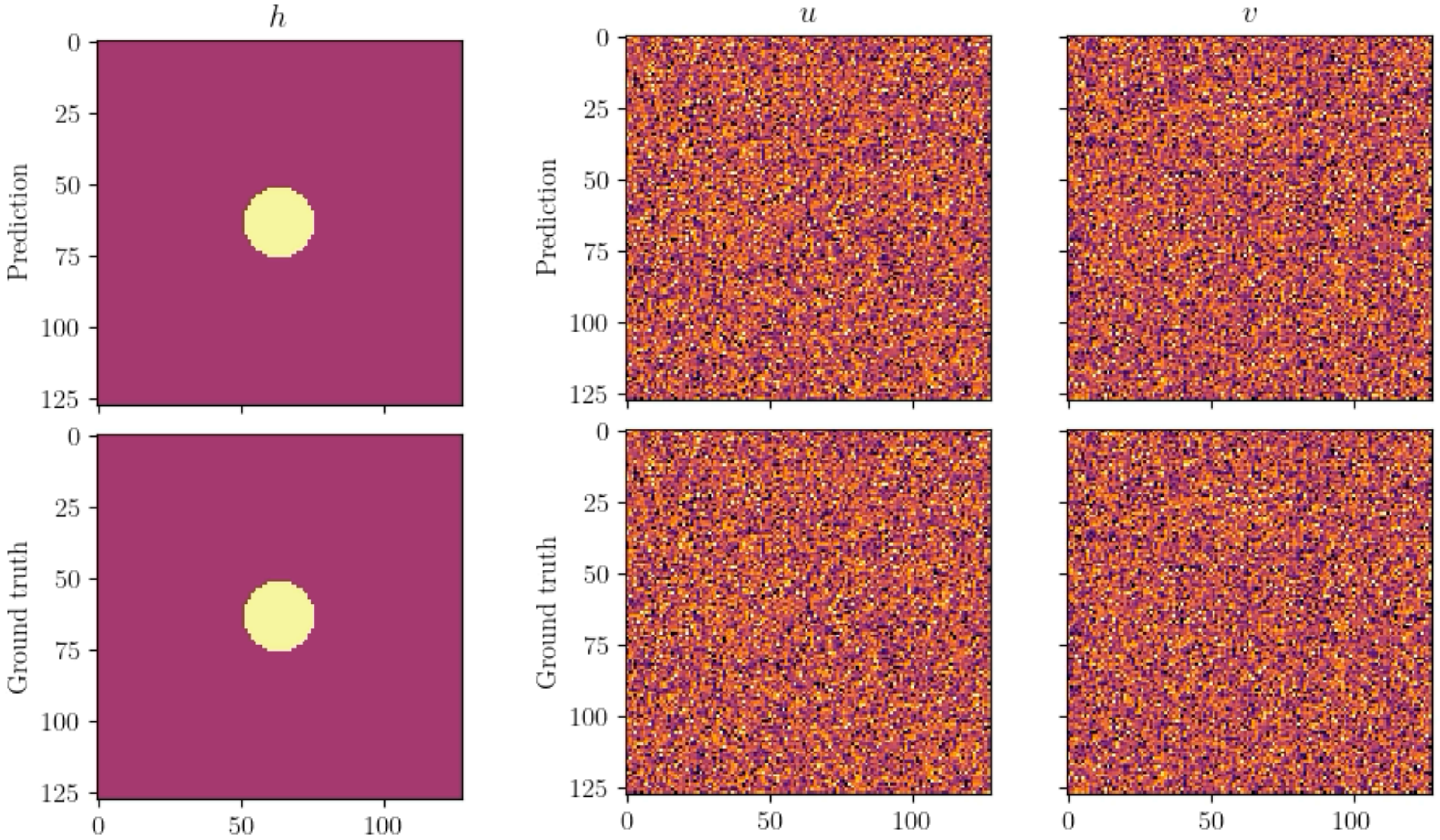
Data in image from PDEBench (Takamoto et al., 2022)

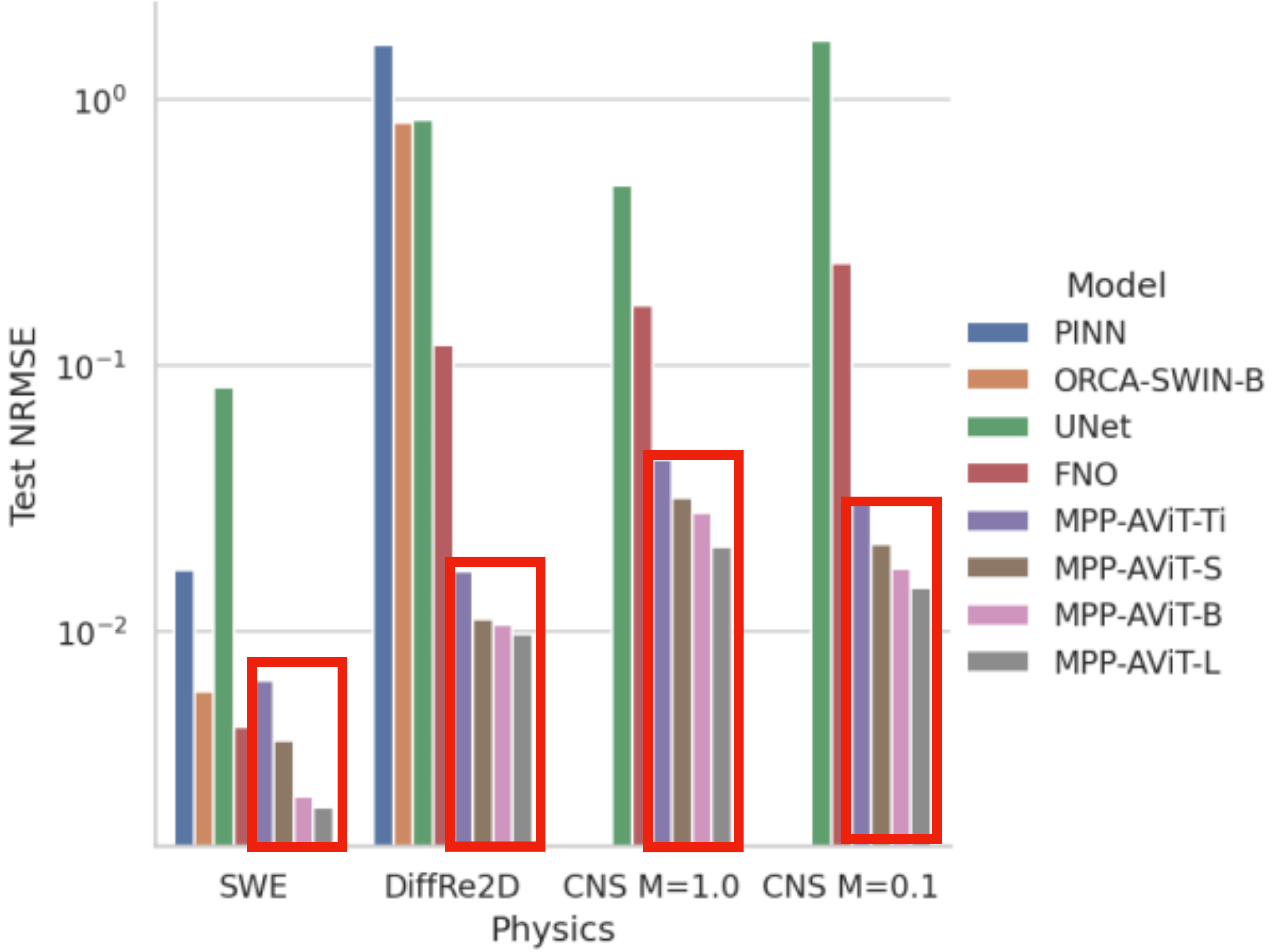
Multiple Physics Pretraining



Pretraining Performance

Does pretraining learn useful representations?





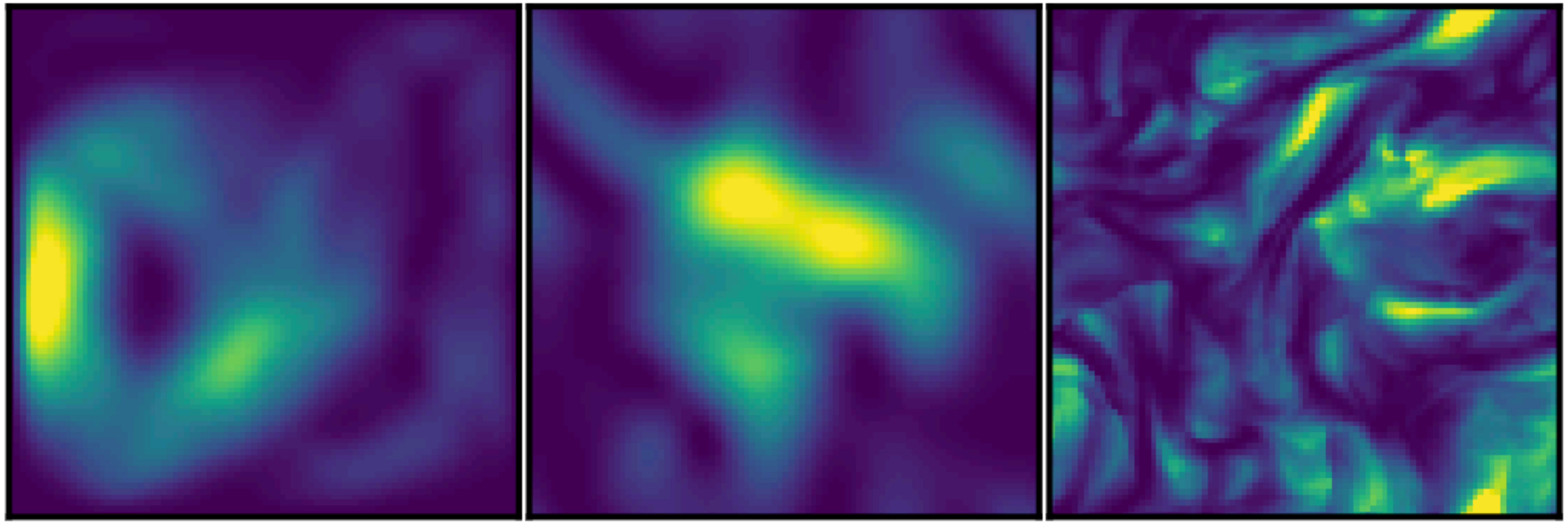
Finetuning Performance

Does pretraining accelerate the learning of new physics?

Not included in training data

Training

“Near” “Far”

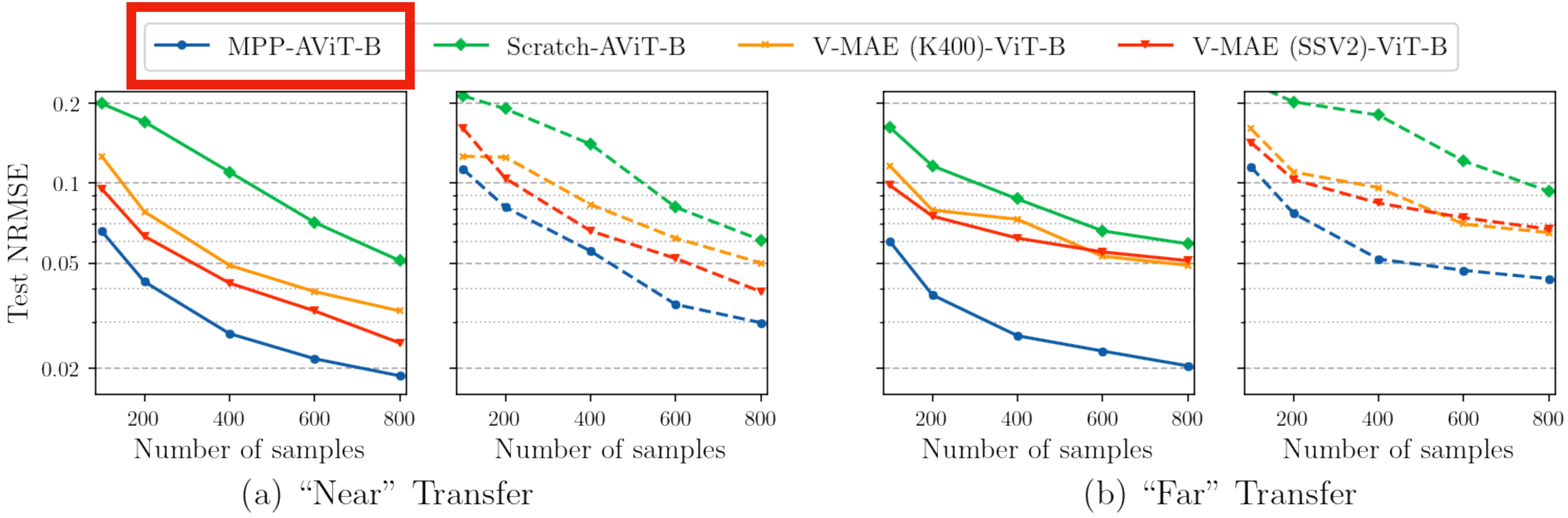


Incompressible Navier-Stokes

Compressible Navier-Stokes Mach=0.1 Highly Diffusive

Compressible Navier-Stokes Mach=1.0 Nearly Inviscid

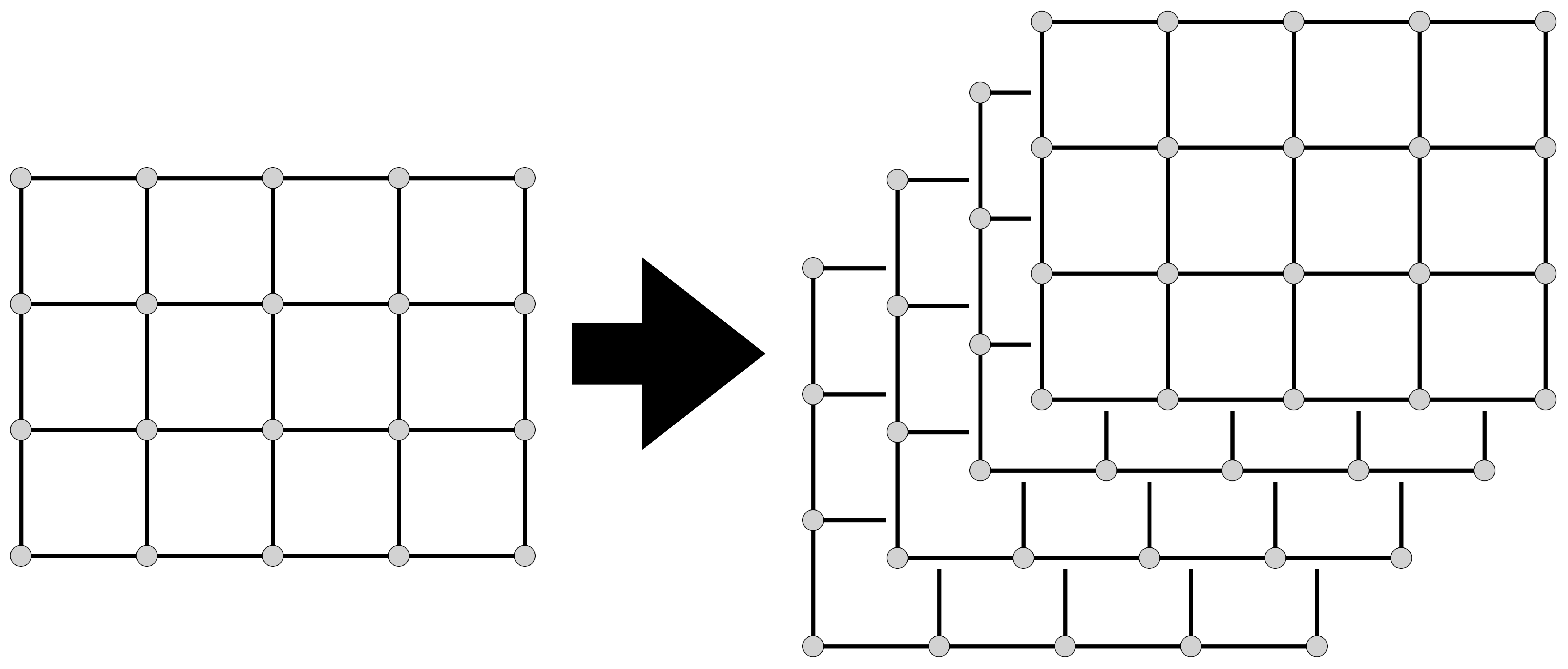
Finetuning Performance



Pretraining on physics data provides an enormous boost over training from scratch or even training on larger volumes of standard video data!

2D->3D Transfer

Kernel Inflation

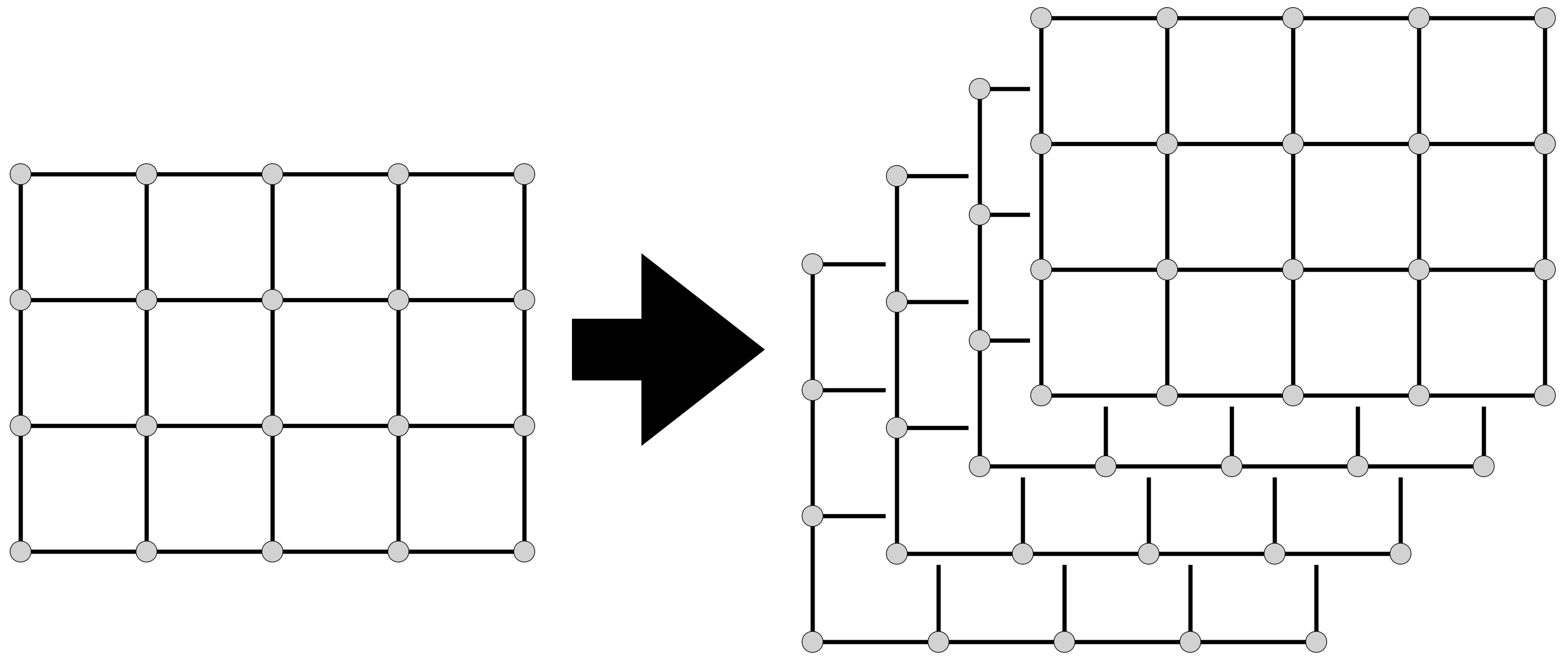


Pretrained 2D Kernel

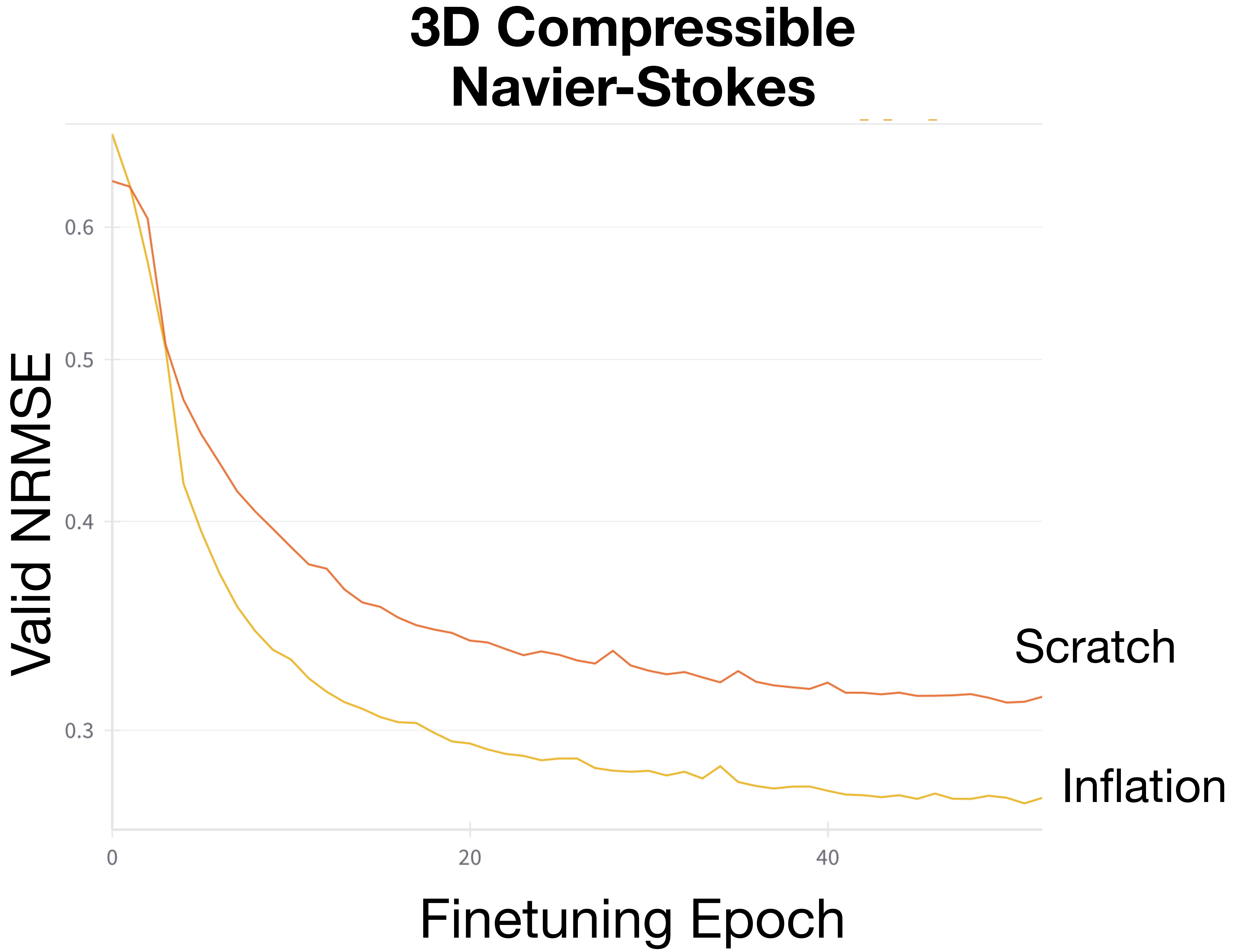
Initialized 3D Kernel

2D->3D Transfer

Kernel Inflation



Pretrained 2D Kernel | **Initialized 3D Kernel**



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