gLaSDI: Parametric physics-informed greedy latent space dynamics identification

6th Annual Sandia MLDL Workshop

July 25th, 2022

Youngsoo Choi

LLNL-PRES-836951

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

Awesome reduced order model team and collaborators


Dylan Copeland


Kevin Huynh


Tony Cheung

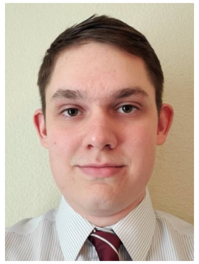

Youngkyu Kim


David Widemann

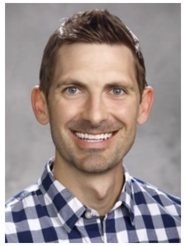

Tarek Zohdi


Jessie Lauzon


Jon Belof


Quincy Huhn


Michael Juhasz


Kevin Carlberg


Peter Brown


Bob Anderson


Sean McBane


Karen Willcox


Rob Rieben


Debojyoti Ghosh

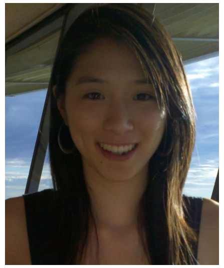

Eric Chin

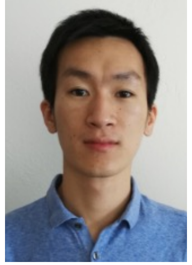

Keo Springer


Dan White


Geoff Oxberry


Trenton Kirchdoerfer

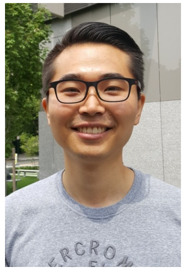

Karen Wang


Xiaolong He


William Fries


Teeratorn Kadeethum


Nikolaos Bouklas


Yeonjong Shin


Saad Khairallah

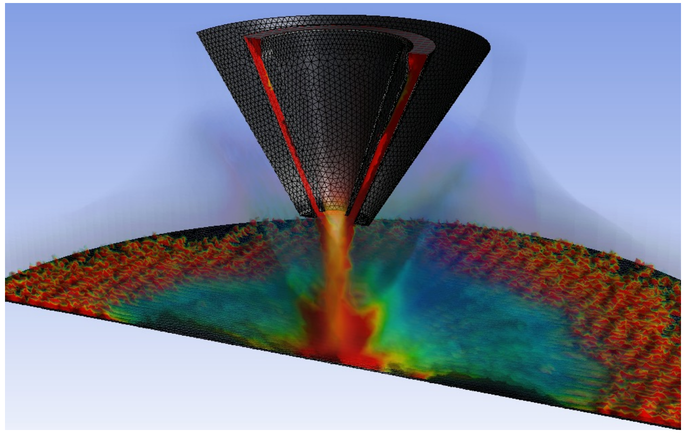

Bedros Afeyan


Jean Ragusa

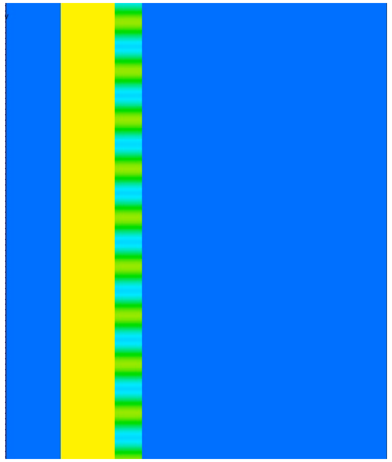

Charles Fredrick Jekel


Xiaoting Zhong

Physical simulations play an important role in modern science

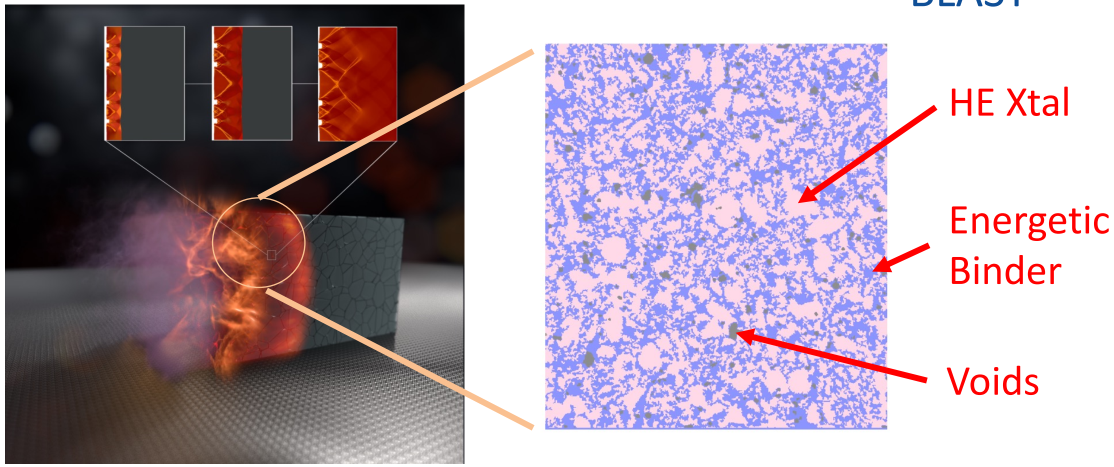


3D Direct energy deposition
(40 minutes on 4 cores) ANSYS

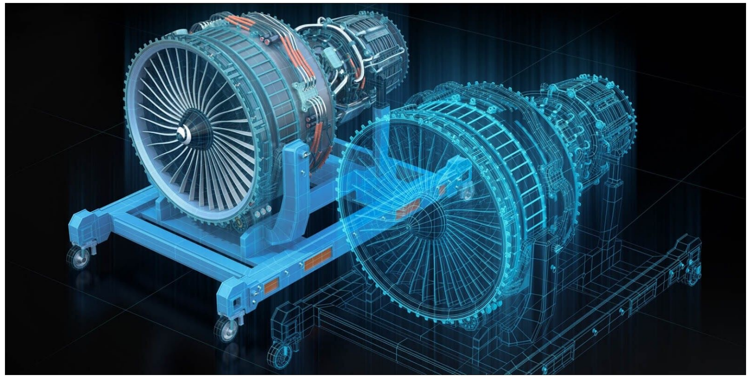


2D Shockwave
(1 hour on 40 cores)
BLAST

3D shaped charge
(23 hours on 96 GPUs)
BLAST



Pore-collapse (1 week on 1024 cores) ALE3D

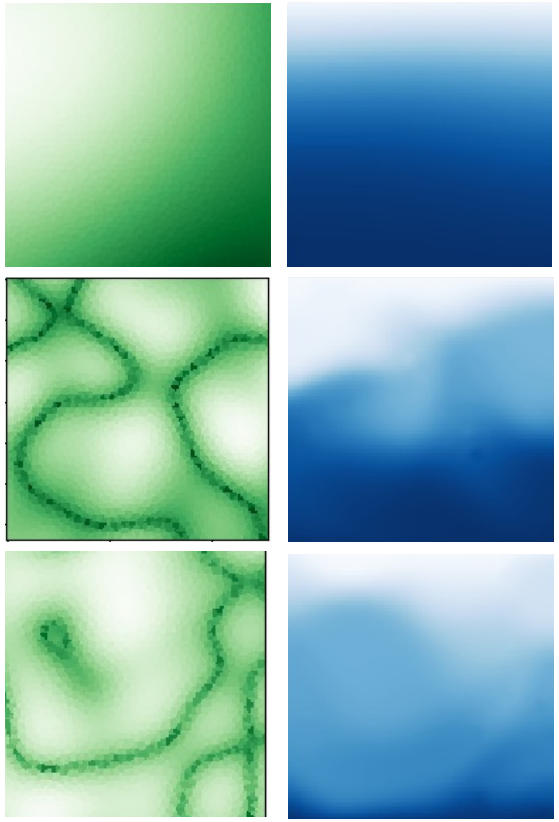


Digital Twin: source from thedigitalspeaker.com

How can you accelerate existing physical simulations with data?

1. Generate Simulation data

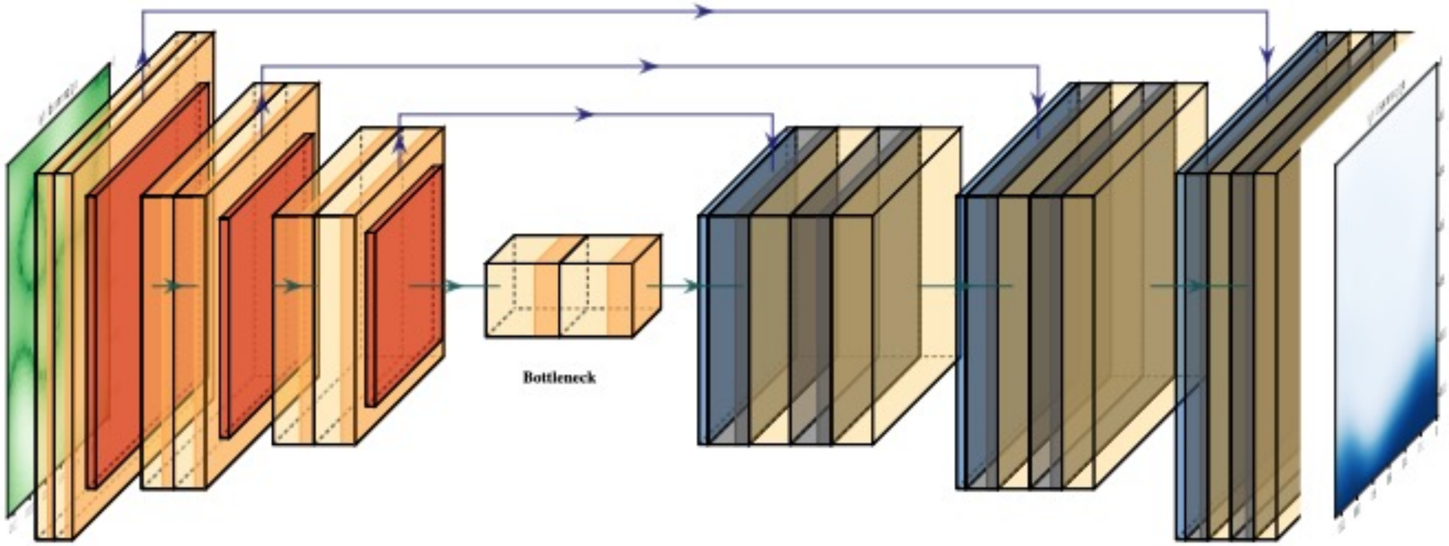
Permeability　Pressure



Input　Output

2. Get the relation between input and output,

e.g., training a neural network



Conditional Generative Adversarial Neural Network

Blackbox approach

*Kadeethum, O'Malley, Fuhg, Choi, Lee, Viswanathan, Bouklas. "A framework for data-driven solution and parameter estimation of PDEs using conditional generative adversarial networks." *Nature Computational Science*, 2021.

How can we get an interpretability? LaSDI

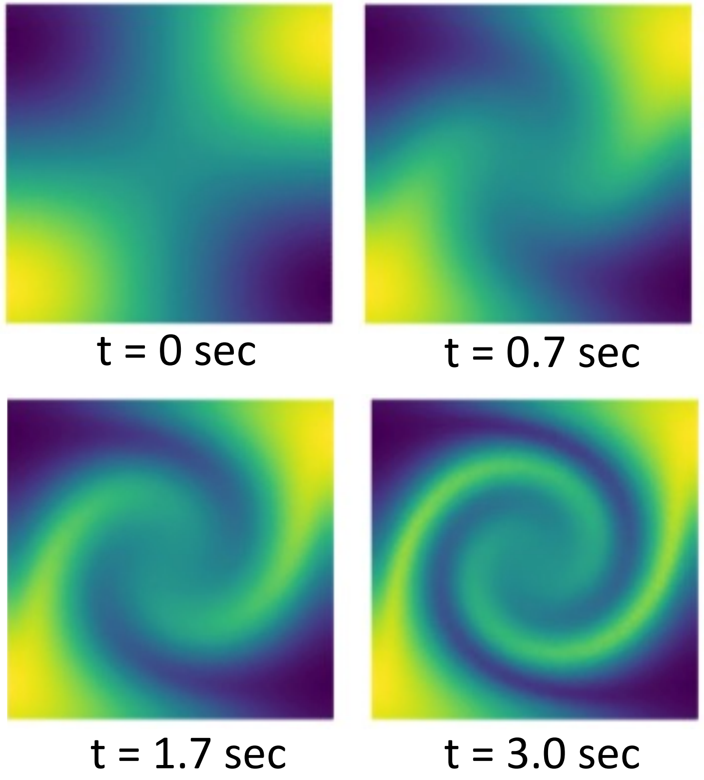
Radial advection:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{u} = \in \Omega = [-1,1]\times[-1,1], \quad t\in[0,3], \qquad \mathbf{v} = \frac{\pi}{2}d[x_2,-x_1]^T, \quad d = (1-x_1^2)^2(1-x_2^2)^2$$

$$u(\mathbf{x},t;\boldsymbol{\mu}) = \mathbf{0} \quad \text{on} \quad \partial\Omega,$$

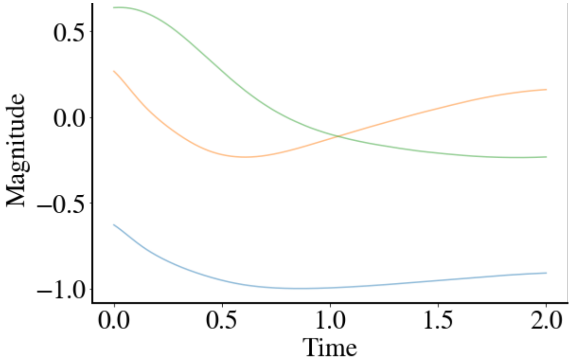
Parameterized initial condition: $u(\mathbf{x},0;\boldsymbol{\mu}) = \sin(w_1x_1)\sin(w_2x_2)$

high dimensional simulation data



compress

Latent space dynamics data
with dimension of 3



Linear compression: POD, SVD, …
Nonlinear compression: Autoencoder

Fit into ODE

$$\frac{d\hat{\boldsymbol{u}}}{dt} = \hat{\boldsymbol{A}}(\boldsymbol{\mu})\Theta(\hat{\boldsymbol{u}})$$

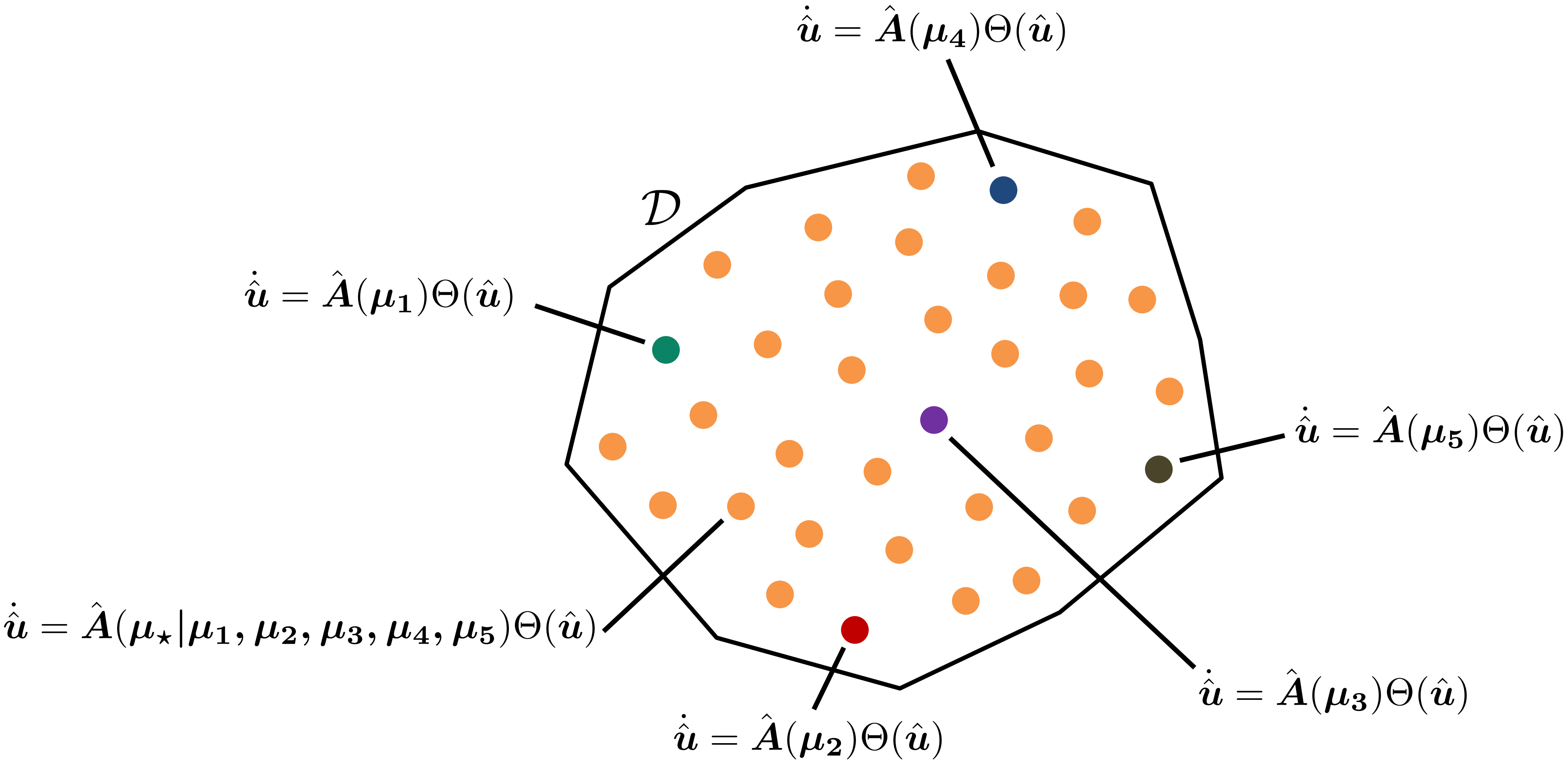
Dynamic mode decomposition (DMD):

$$\frac{d\hat{\boldsymbol{u}}}{dt} = \hat{\boldsymbol{A}}(\boldsymbol{\mu})\hat{\boldsymbol{u}}$$

Operator Inference (OpInf):

$$\frac{d\hat{\boldsymbol{u}}}{dt} = \hat{\boldsymbol{A}}(\boldsymbol{\mu})\hat{\boldsymbol{u}} + \hat{\boldsymbol{H}}(\hat{\boldsymbol{u}}\otimes\hat{\boldsymbol{u}})$$

Parameterized latent space dynamics identification (LaSDI)



Fries, He, Choi, "Lasdi: Parametric latent space dynamics identification." arXiv:2203.02076, 2022.

Interpretable

Performance of LaSDI to radial advection problem

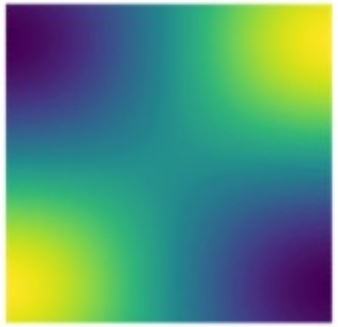
Radial advection:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{u} =\in \Omega = [-1,1]\times[-1,1], \quad t\in[0,3], \qquad \mathbf{v} = \frac{\pi}{2}d[x_2, -x_1]^T, \quad d = (1-x_1^2)^2(1-x_2^2)^2$$

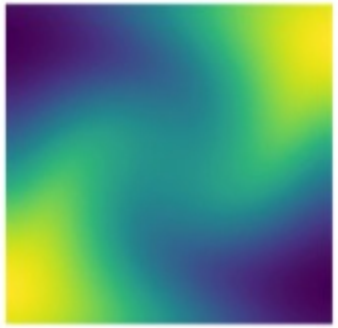
$$u(\mathbf{x}, t; \boldsymbol{\mu}) = \mathbf{0} \quad \text{on} \quad \partial\Omega,$$

Parameterized initial condition: $u(\mathbf{x}, 0; \boldsymbol{\mu}) = \sin(w_1 x_1)\sin(w_2 x_2)$

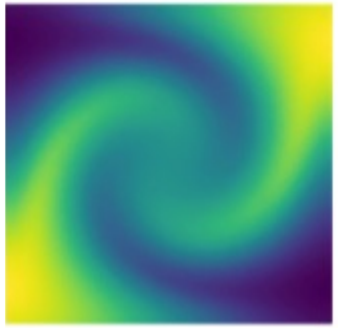
High dimensional simulation data



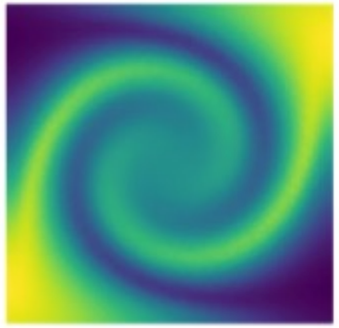
t = 0 sec



t = 0.7 sec

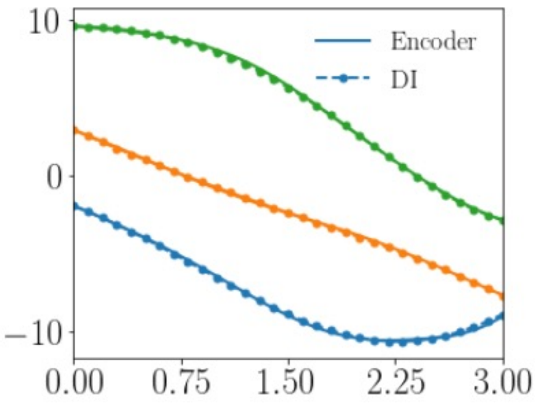


t = 1.7 sec

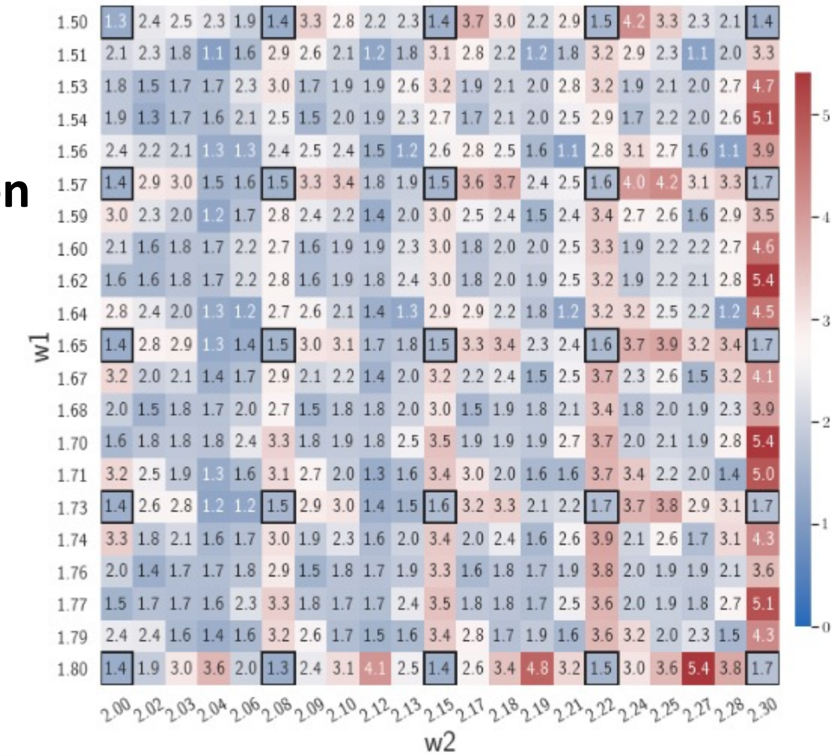


t = 3.0 sec

Latent space dynamics identification
with a dimension of 3

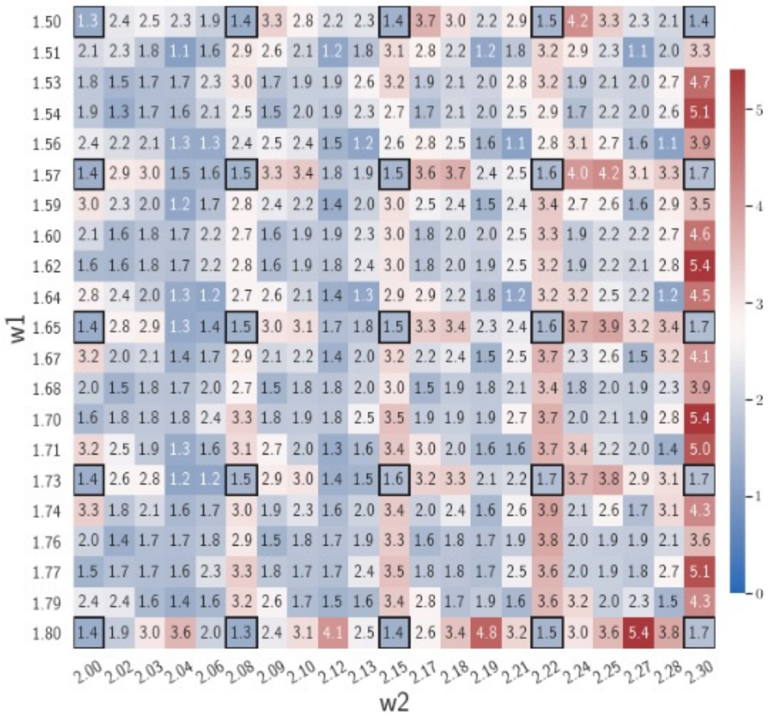


Maximum relative error:
5.4% with 25 uniformly sampled training points
Speed-up of 200x



Is uniform sampling enough? No, so we need physics-informed greedy sampling!

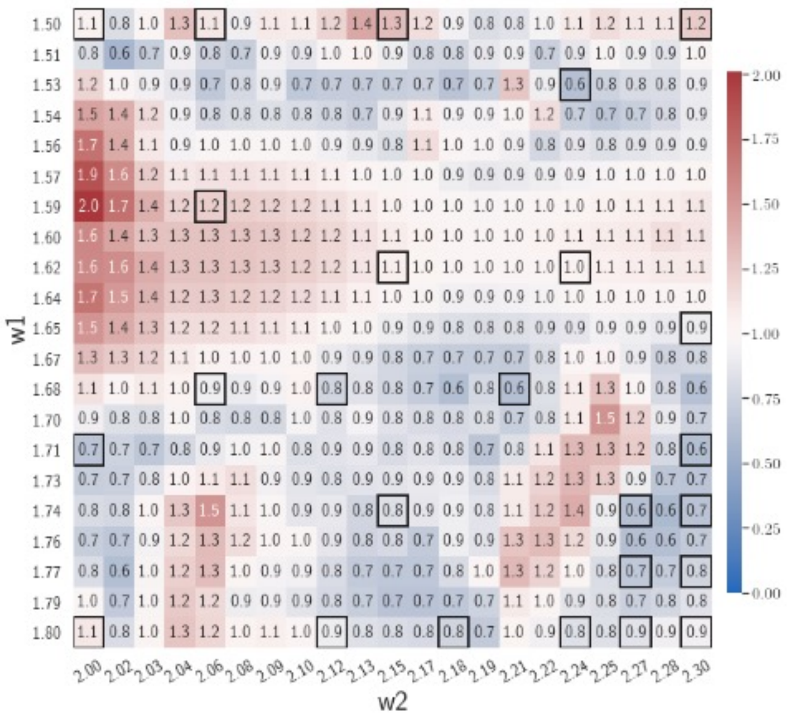
Uniform sampling



Maximum relative error:

5.4% with 25 uniformly sampled training points

Physics-informed greedy sampling



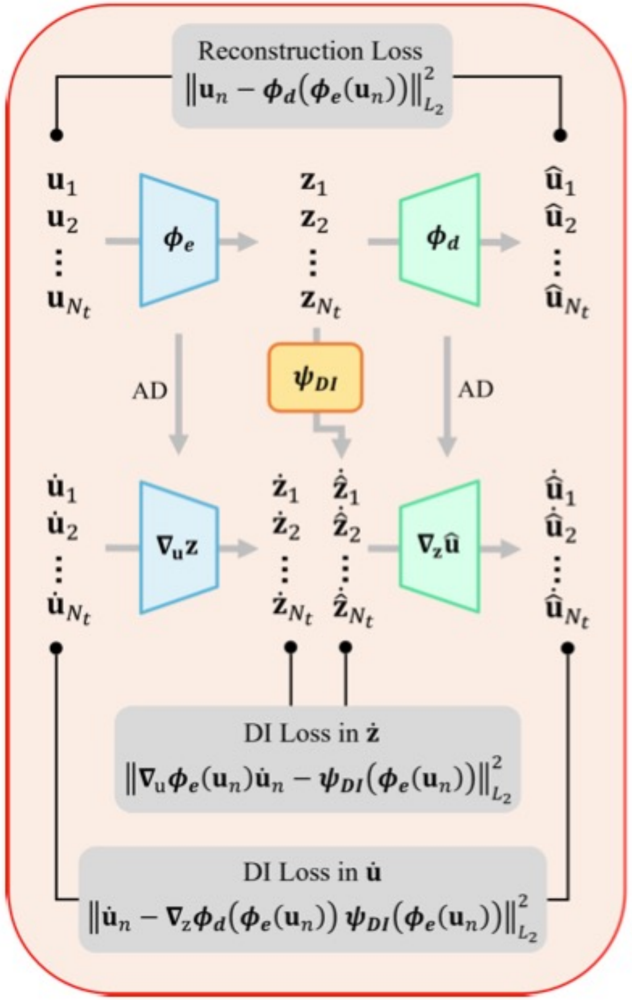
Maximum relative error:

2.0% with 25 greedy sampling points

*He, Choi, Fries, Belof, Chen. ”gLaSDI: Parametric Physics-informed Greedy Latent Space Dynamics Identification." arXiv:2204.12005. 2022.

gLaSDI: physics-informed greedy latent space dynamics identification*

Interactive Auto-DI training

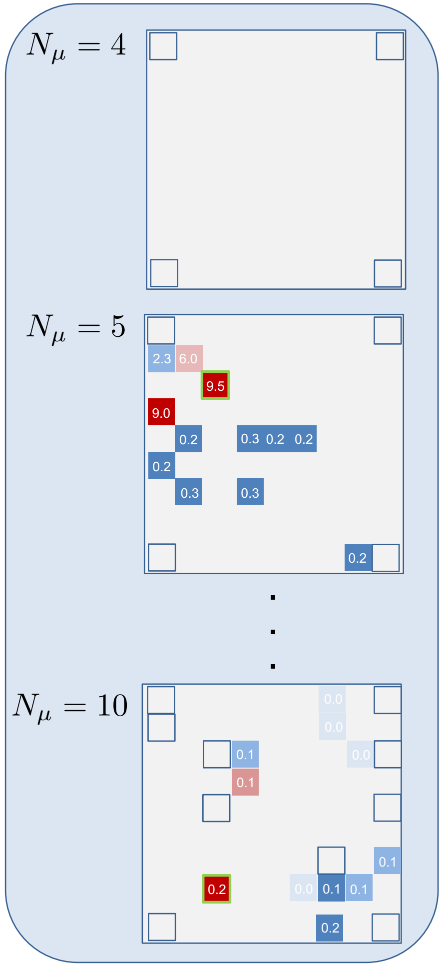


While $N_\mu \le N_\mu^{max}$:

- Model Training
- Sampling:
  - Random Selection
  - Error Indicator
- $N_\mu \leftarrow N_\mu + 1$

End

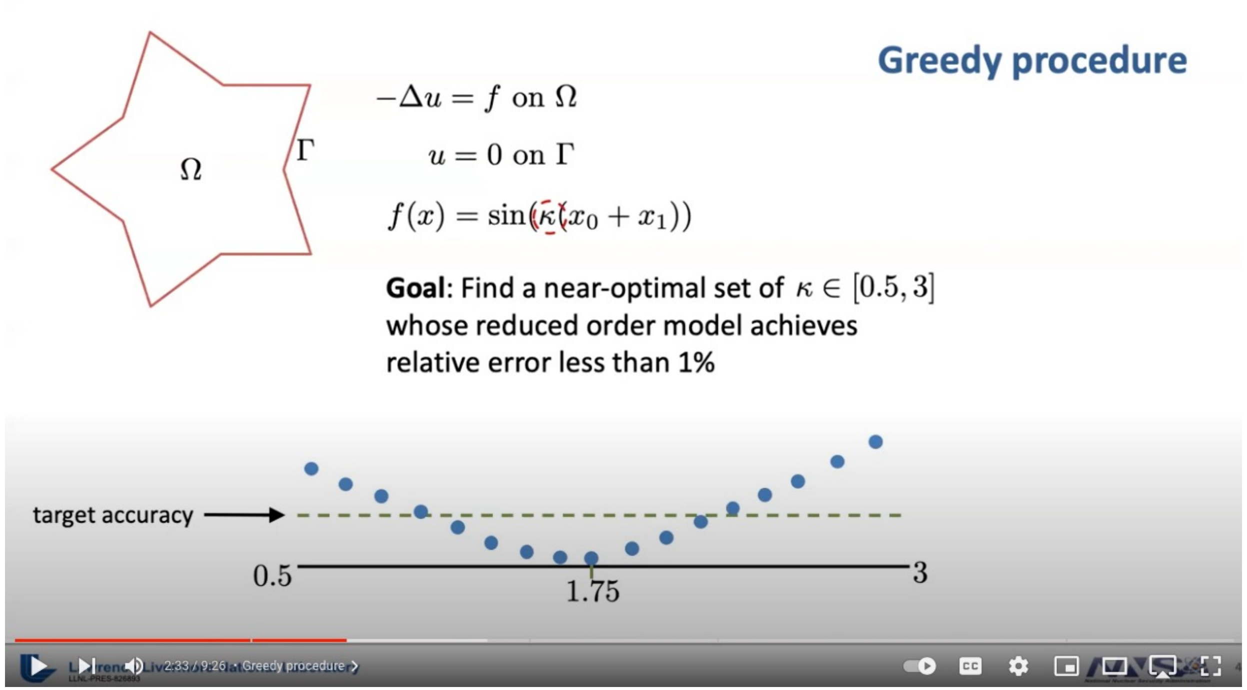
Greedy Sampling Iteration

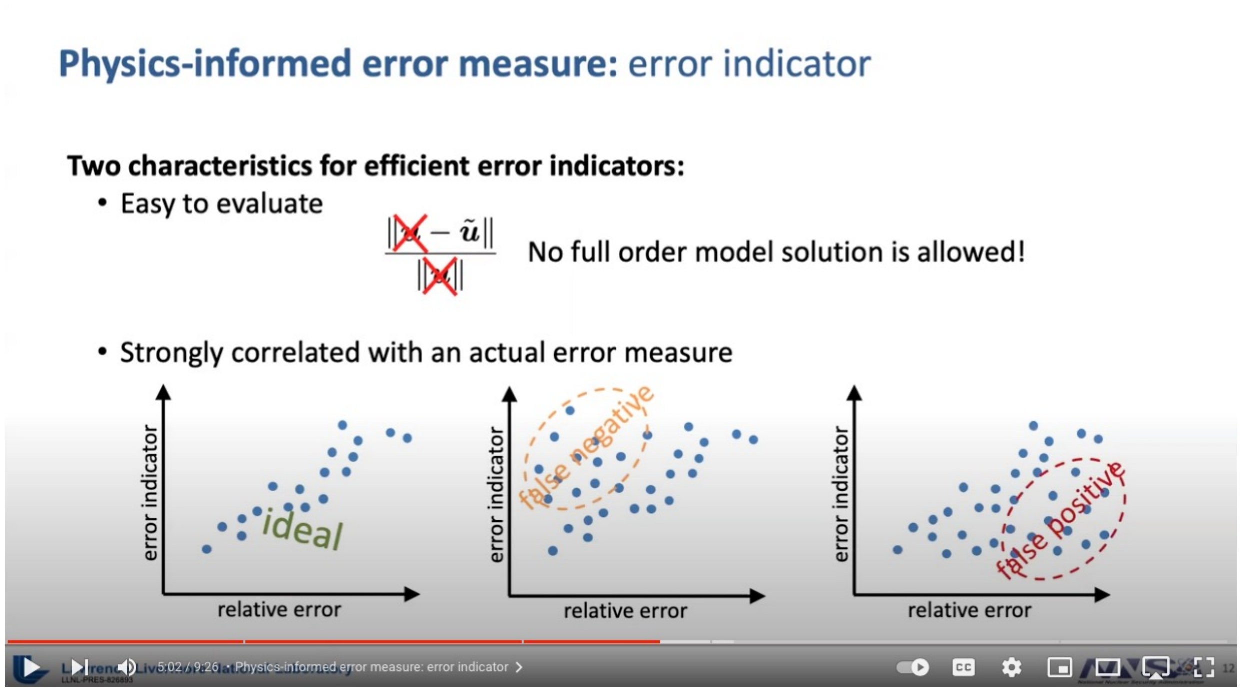


*He, Choi, Fries, Belof, Chen. "gLaSDI: Parametric Physics-informed Greedy Latent Space Dynamics Identification." arXiv:2204.12005. 2022

Curious about the physics-informed greedy procedure?

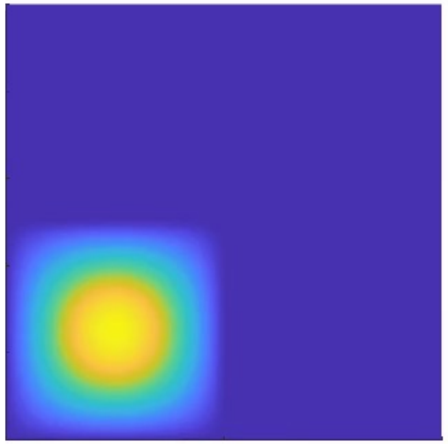
- Watch this YouTube video (less than 10minutes) : https://youtu.be/A5JlIXRHxrI





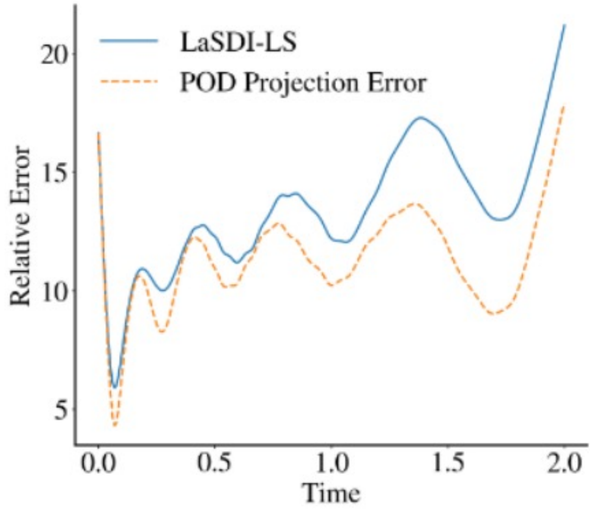
Interpretable

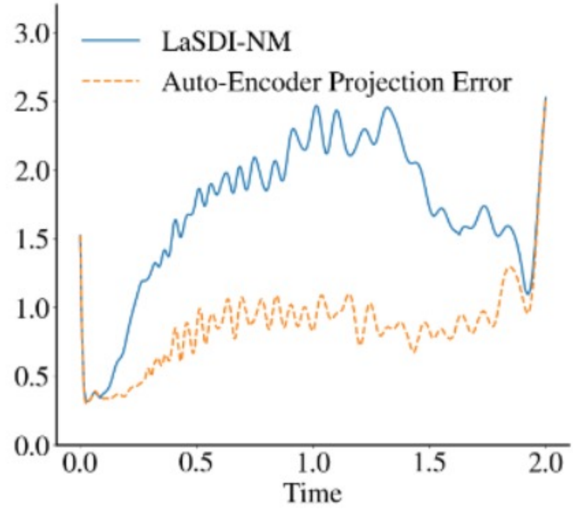
Does linear compression always work? No
Benefit of nonlinear compression



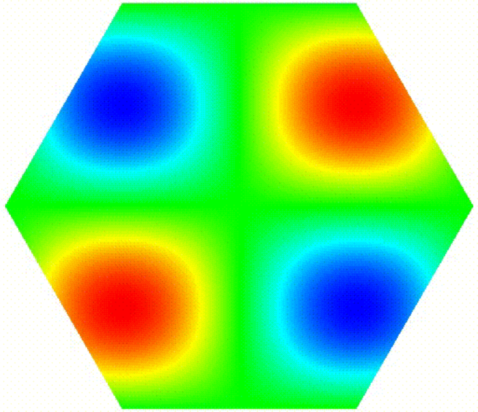
2D Burgers

☺ Better projection error



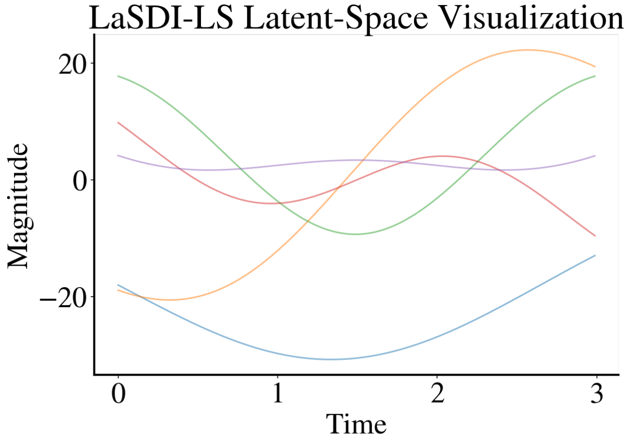


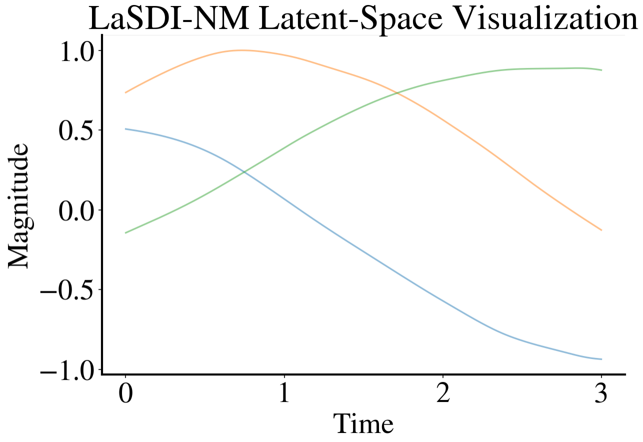
Linear compression vs. **Nonlinear compression**



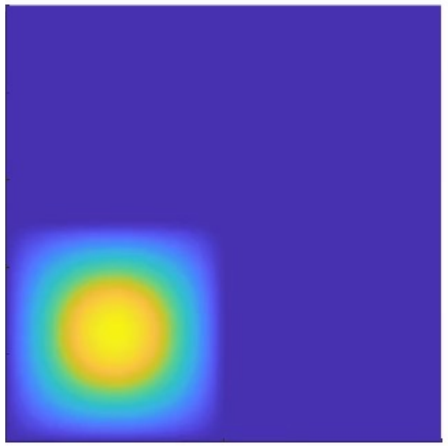
radial advection

☺ Simpler latent space dynamics





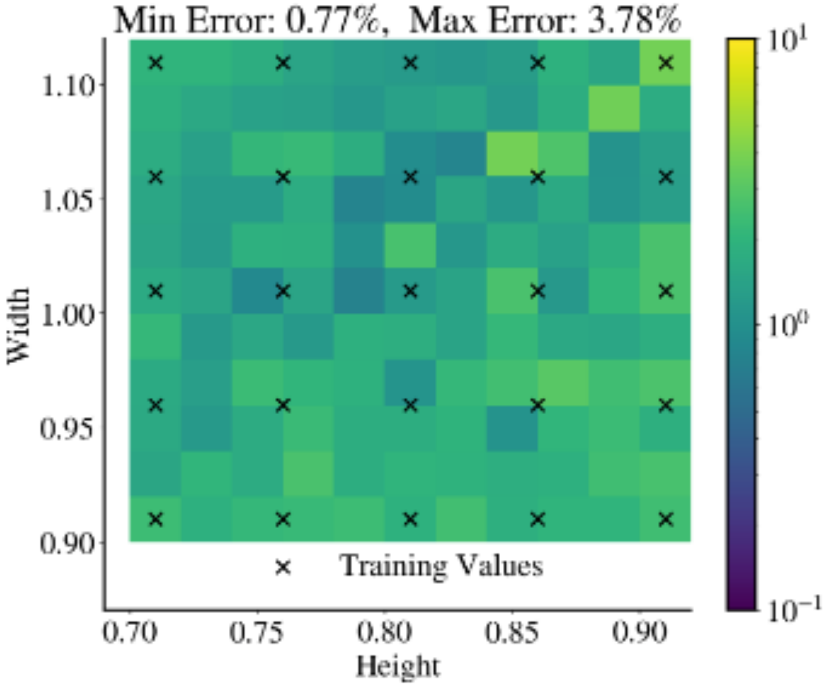
Nonlinear compression outperforms!



2D Burgers

advection-dominated

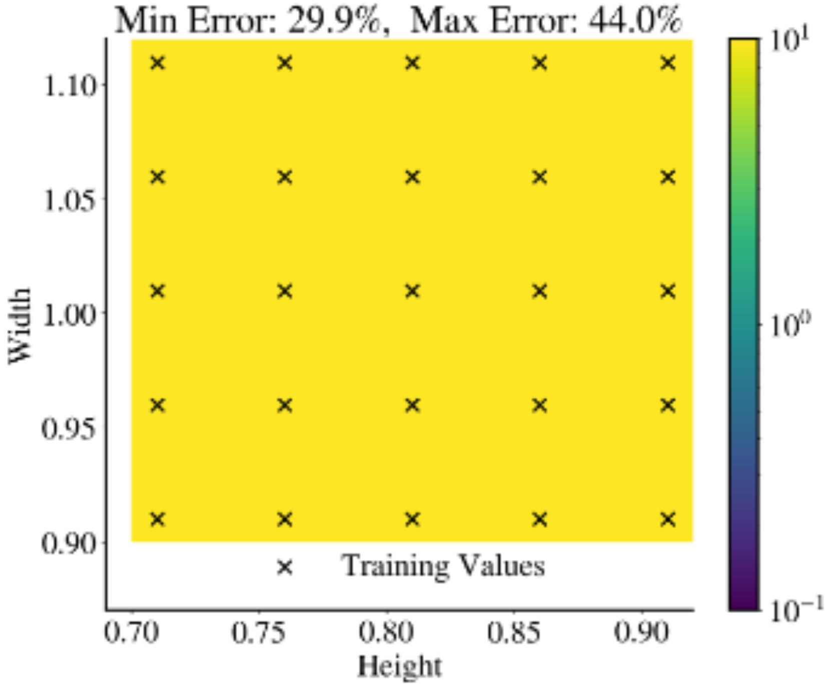
Nonlinear manifold



Latent space dimension of **three**

Cubic ODE for latent space dynamics model

Linear subspace



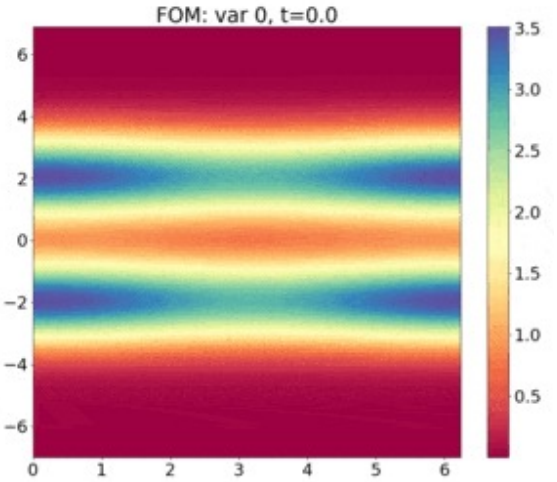
Latent space dimension of **five**

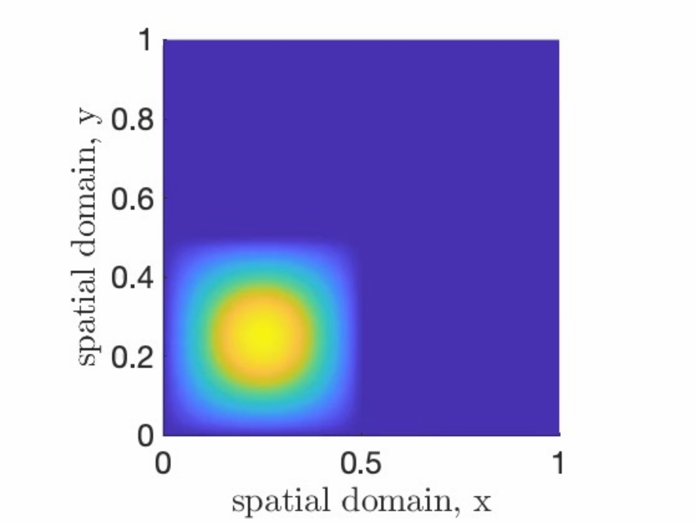
Linear ODE for latent space dynamics model

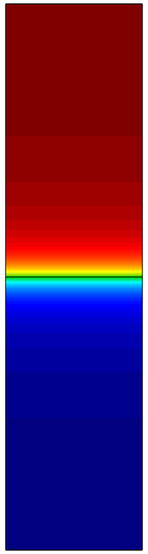
*Fries, He, Choi, "LaSDI: Parametric latent space dynamics identification." arXiv:2203.02076, 2022.

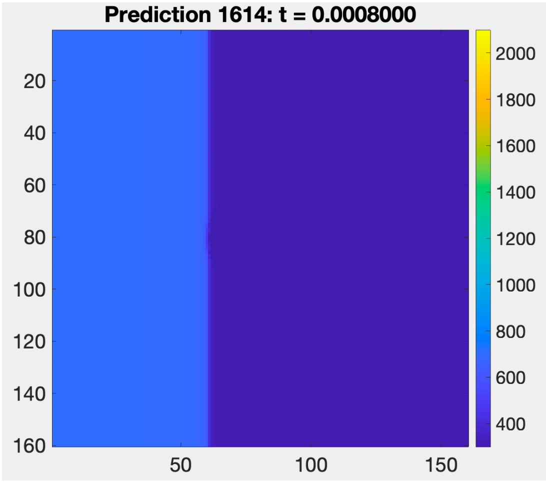
*He, Choi, Fries, Belof, Chen. "gLaSDI: Parametric Physics-informed Greedy Latent Space Dynamics Identification." arXiv:2204.12005. 2022

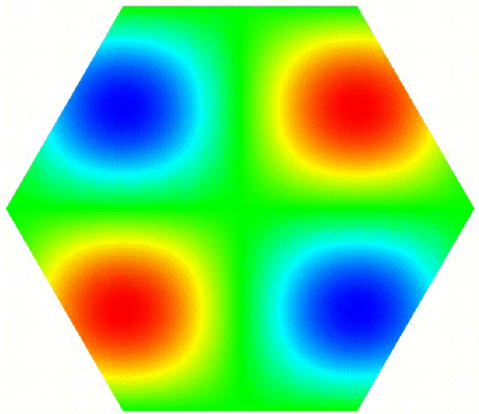
Questions? Email choi15@llnl.gov

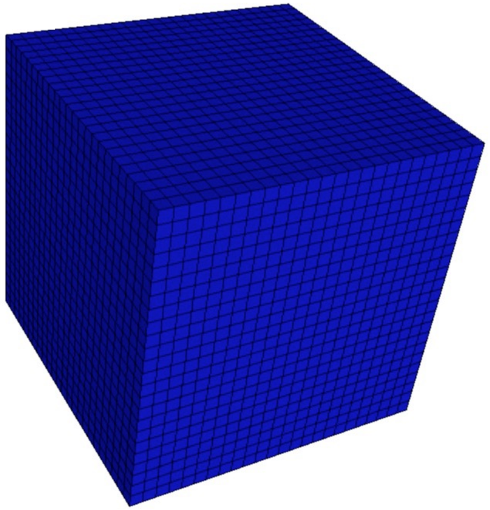












Lawrence Livermore National Laboratory