gLaSDI: Parametric physics-informed greedy latent space dynamics identification

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Awesome reduced order model team and collaborators
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](image1.png) | ![Output](image2.png) |

2. Get the relation between input and output, e.g., training a neural network

- Conditional Generative Adversarial Neural Network

*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

Dynamic mode decomposition (DMD):
\[ \frac{d\hat{u}}{dt} = \hat{A}(\mu)\hat{u} \]

Operator Inference (OpInf):
\[ \frac{d\hat{u}}{dt} = \hat{A}(\mu)\hat{u} + \hat{H}(\hat{u} \otimes \hat{u}) \]

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

Parameterized initial condition: \[ u(x, 0; \mu) = \sin(w_1 x_1)\sin(w_2 x_2) \]

High dimensional simulation data

Latent space dynamics data with dimension of 3

Fit into ODE

Linear compression: POD, SVD, ...
Nonlinear compression: Autoencoder
Parameterized latent space dynamics identification (LaSDI)

\[ \dot{\hat{u}} = \hat{A}(\mu_1)\Theta(\hat{u}) \]

\[ \dot{\hat{u}} = \hat{A}(\mu_2)\Theta(\hat{u}) \]

\[ \dot{\hat{u}} = \hat{A}(\mu_3)\Theta(\hat{u}) \]

\[ \dot{\hat{u}} = \hat{A}(\mu_4)\Theta(\hat{u}) \]

\[ \dot{\hat{u}} = \hat{A}(\mu_5)\Theta(\hat{u}) \]

Fries, He, Choi, “Lasdi: Parametric latent space dynamics identification.” arXiv:2203.02076, 2022.
Performance of LaSDI to radial advection problem

Radial advection:
\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{u} = 0 \quad \Omega = [-1, 1] \times [-1, 1], \quad t \in [0, 3],
\]
\[
\mathbf{v} = \frac{\pi}{2} d[x_2, -x_1]T, \quad d = (1 - x_1^2)^2(1 - x_2^2)^2
\]
\[
u(x, t; \mu) = 0 \quad \text{on} \quad \partial \Omega,
\]
Parameterized initial condition: \( u(x, 0; \mu) = \sin(w_1 x_1)\sin(w_2 x_2) \)

High dimensional simulation data

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**

*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 10 minutes): [https://youtu.be/A5JIIXRHxrl](https://youtu.be/A5JIIXRHxrl)
Does linear compression always work? No

Benefit of nonlinear compression

😊 Better projection error

2D Burgers

😊 Simpler latent space dynamics

radial advection

Linear compression vs. Nonlinear compression

LaSDI-LS Latent-Space Visualization

LaSDI-NM Latent-Space Visualization
Nonlinear compression outperforms!

Nonlinear manifold

Min Error: 0.77%, Max Error: 3.78%

Linear subspace

Min Error: 29.9%, Max Error: 44.0%

2D Burgers advection-dominated

Latent space dimension of three

Cubic ODE for latent space dynamics model

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
