Hyper-reduced nonlinear manifold reduced order model

Physics-constrained learning III

ML4I

August 12, 2021

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Lawrence Livermore National Laboratory

Awesome team


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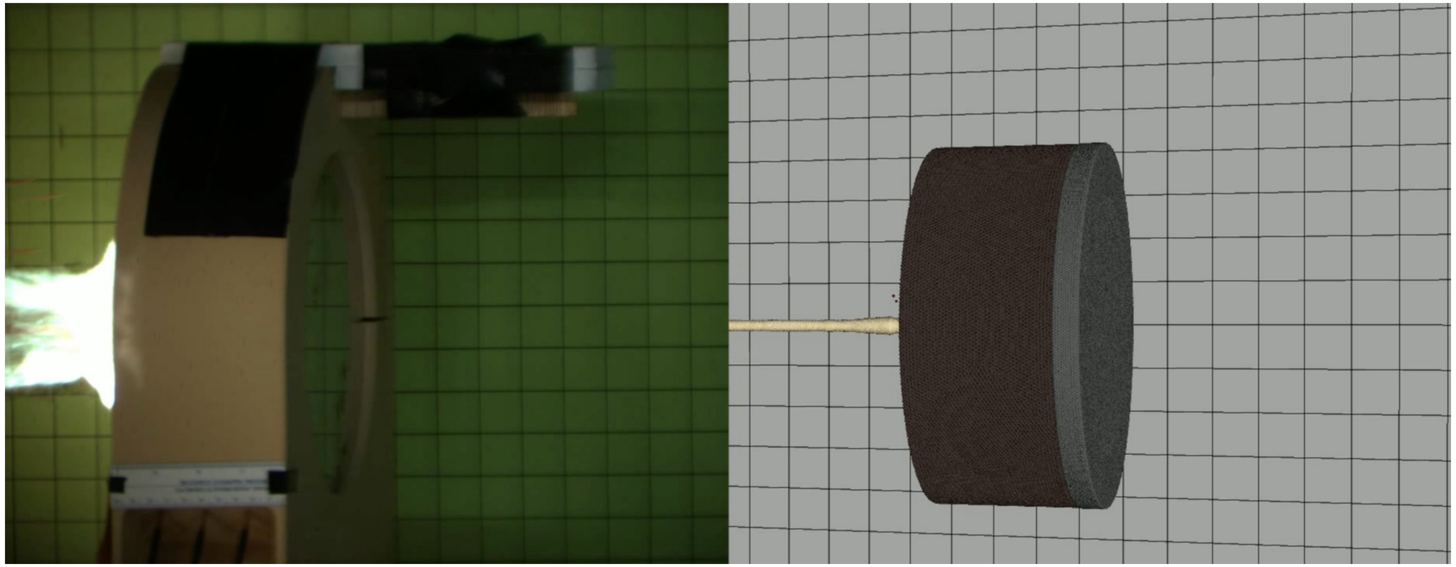
David Widemann


Tarek Zohdi

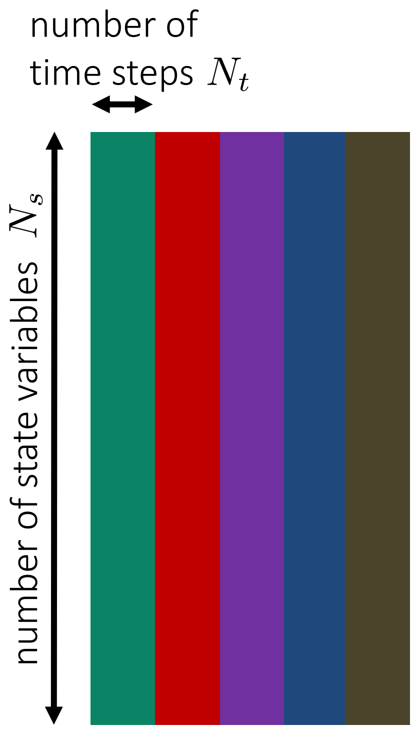
Smooth Particle Hydrodynamic (SPH) modeling for jet [courtesy: Karen Wang]

One forward simulation:
- 10.1 million particles
- 1,440 processors
- 178 hours (7.4 days)



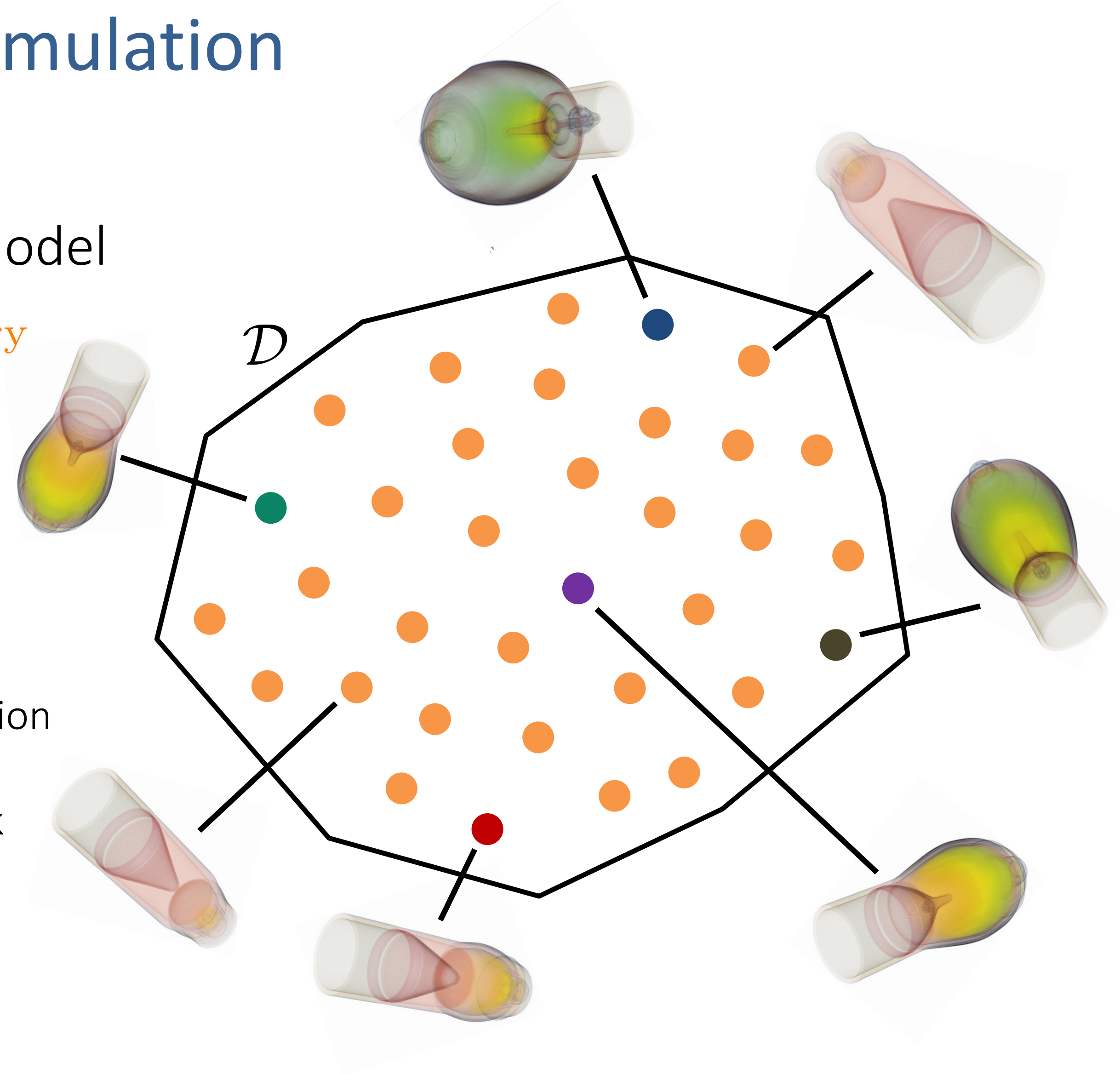
Approach: Data-driven physical simulation

1. *Collect data*: solve FOM for $\boldsymbol{\mu} \in \mathcal{D}_{\text{sample}}$
2. *Machine learning*: build a reduced order model
3. *Accelerate* physical simulation, $\boldsymbol{\mu} \in \mathcal{D}_{\text{query}}$



- Principal component analysis
- Tucker decomposition
- Canonical Polyadic decomposition
- Autoencoder
- Generative adversarial network
- Gaussian processes

Intrusive vs. **non-intrusive**

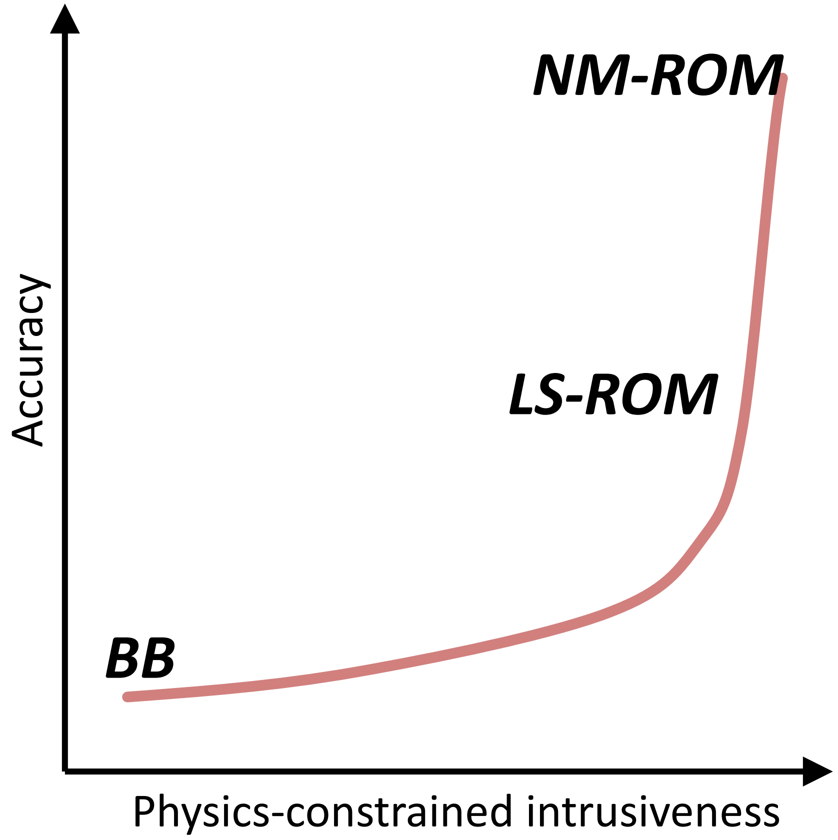


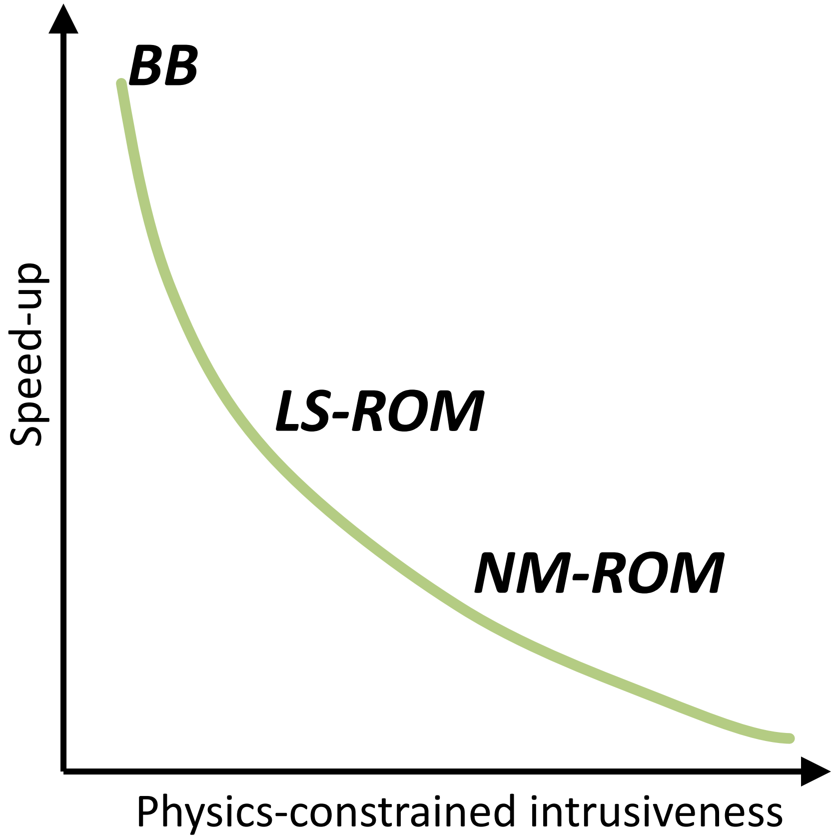
Category of reduced order models via level of intrusiveness

BB: Black-box approach

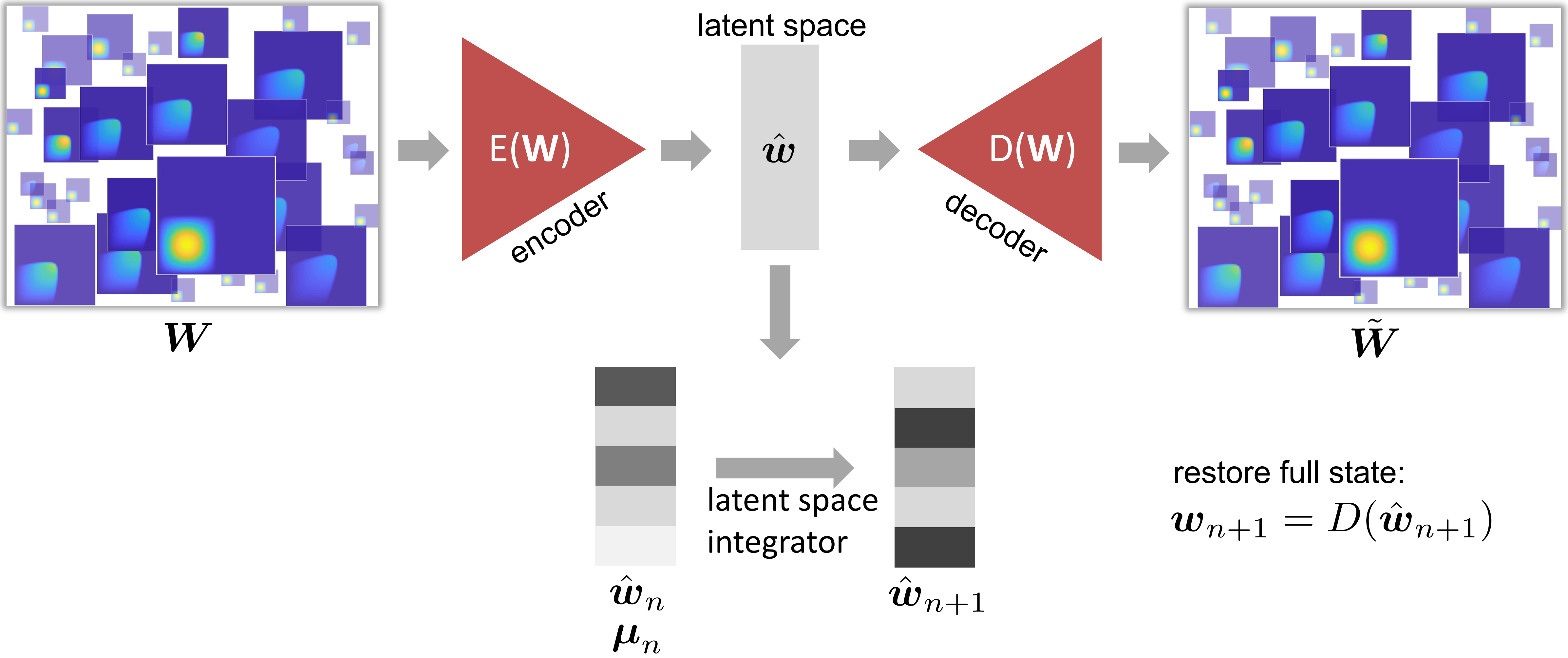
LS-ROM: Linear subspace ROM

NM-ROM: Nonlinear manifold ROM





Black box approach, Deep Fluid: Nonlinear manifold learning*



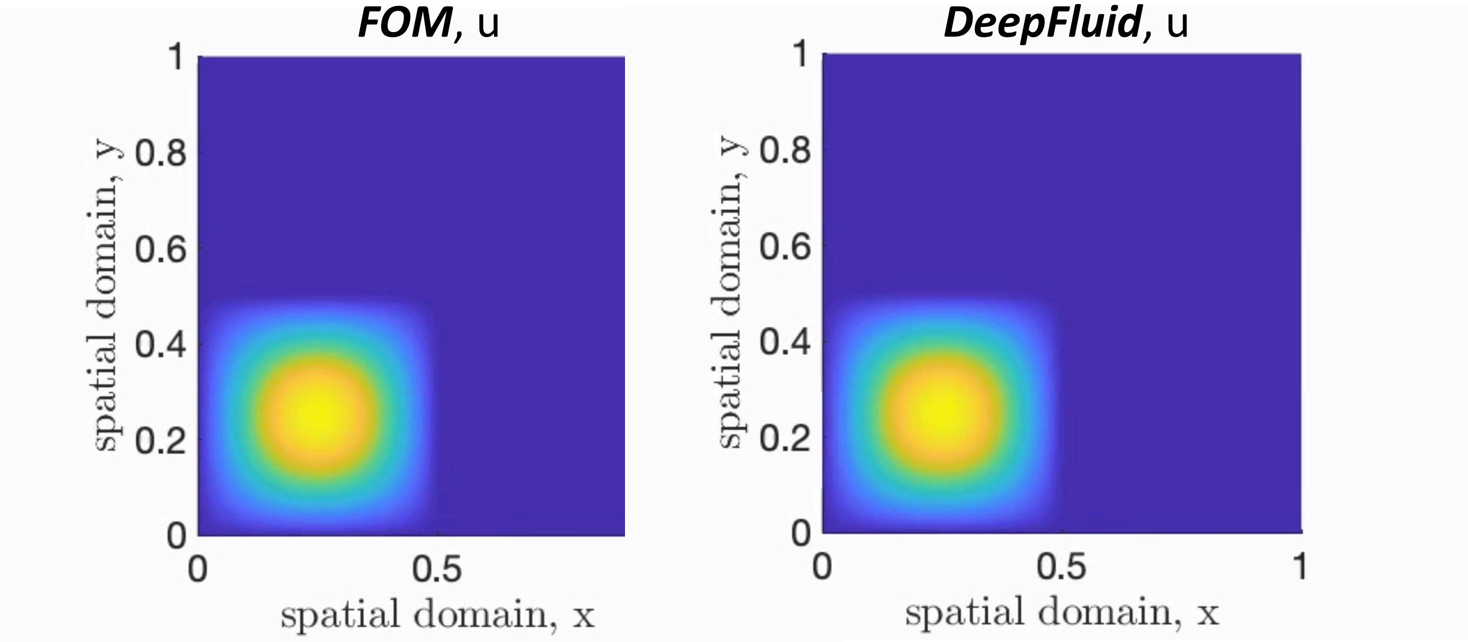
restore full state:

$$w_{n+1} = D(\hat{w}_{n+1})$$

*Kim, Byungsoo, et al. "Deep fluids: A generative network for parameterized fluid simulations." *Computer Graphics Forum*. Vol. 38. No. 2. 2019.

Results: Burgers' equation* [with Youngkyu Kim, David Widemann, Tarek Zohdi]

$$\frac{\partial u}{dt} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \qquad \frac{\partial v}{dt} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \qquad Re = 1/\nu = 10,000$$



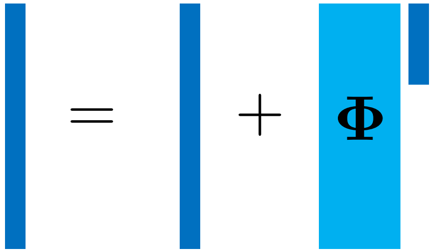
method	DeepFluid
max. rel. error (%)	38.6
speed-up	119

*Kim, Choi, Widemann, and Zohdi, "Efficient nonlinear manifold reduced order model." *Workshop on machine learning for engineering modeling, simulation and design @ NeurIPS 2020*

Projection-based linear subspace reduced order model

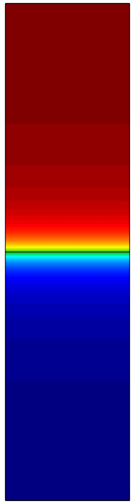
- Governing equation: $\dfrac{d\boldsymbol{w}}{dt} = \boldsymbol{f}(\boldsymbol{w}, t; \boldsymbol{\mu}), \qquad \boldsymbol{w}, \boldsymbol{f} \in \mathbb{R}^{N_s}$
- Solution approximation:

$$\boldsymbol{w} \approx \tilde{\boldsymbol{w}} = \boldsymbol{w}_{\text{ref}} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}, \quad \boldsymbol{\Phi} \in \mathbb{R}^{N_s \times n_s}, \quad n_s \ll N_s$$



- Reduced system after Galerkin projection: $\dfrac{d\hat{\boldsymbol{w}}}{dt} = \boldsymbol{\Phi}^T \boldsymbol{f}(\boldsymbol{w}_{\text{ref}} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}, t; \boldsymbol{\mu})$
- Backward Euler time integrator: $\hat{\boldsymbol{w}}_n = \hat{\boldsymbol{w}}_{n-1} + \Delta t \underbrace{\boldsymbol{\Phi}^T \boldsymbol{f}}_{\text{Scales with FOM size: } \mathbb{R}^{N_s}}(\boldsymbol{w}_{\text{ref}} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}, t; \boldsymbol{\mu})$

Successful applications of linear subspace ROM



Rayleigh–Taylor

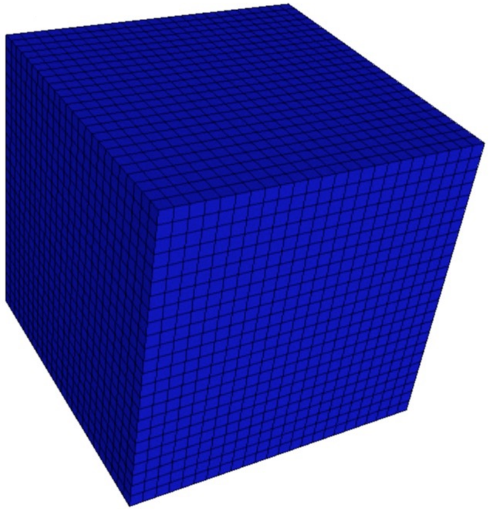
Kinematic dofs: 8,514

Energy dofs: 4,096

Wall-clock time: 127 sec

Relative error & speedup

Position: 5.3e-5
Velocity: 7.8e-3
Energy : 243e-5
Speedup: 14.6



Sedov blast

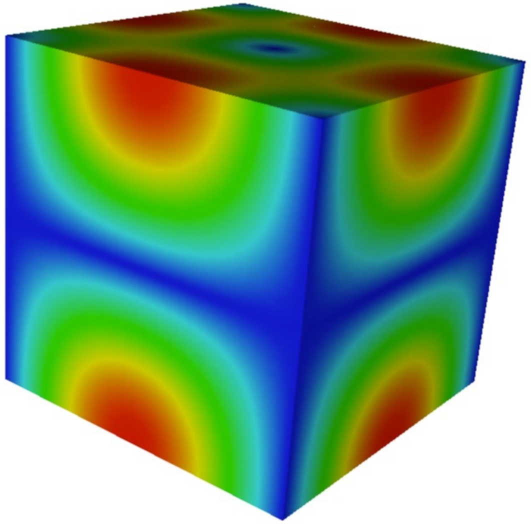
Kinematic dofs: 14,739

Energy dofs: 4,096

Wall-clock time: 191 sec

Relative error & speedup

Position: 2.2e-5
Velocity: 2.2e-4
Energy : 2.3e-4
Speedup: 22.8



Taylor–Green

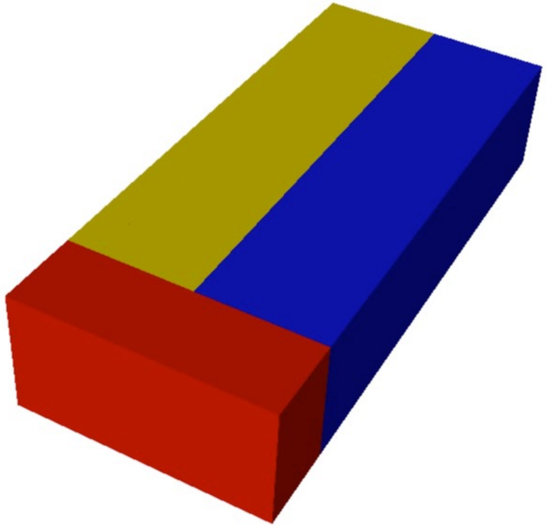
Kinematic dofs: 14,739

Energy dofs: 4,096

Wall-clock time: 170 sec

Relative error & speedup

Position: 1.8e-8
Velocity: 1.1e-6
Energy : 1.0e-7
Speedup: 31.2



Triple-point problem

Kinematic dofs: 38,475

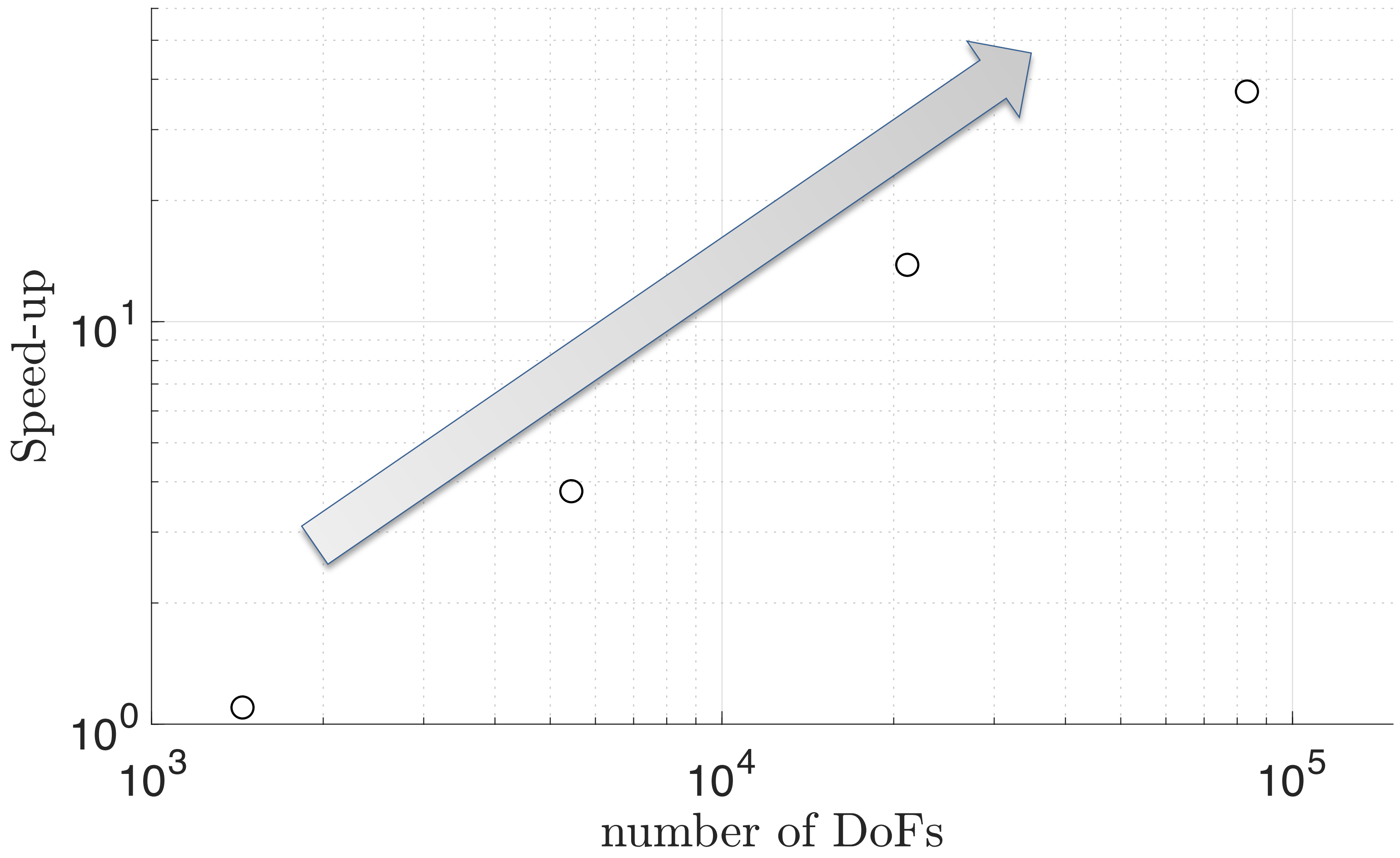
Energy dofs: 10,752

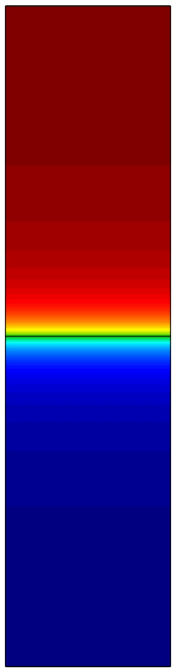
Wall-clock time: 122 sec

Relative error & speedup

Position: 3.1e-5
Velocity: 8.1e-4
Energy : 2.8e-4
Speedup: 87.8

Speedup increases as problem size increases

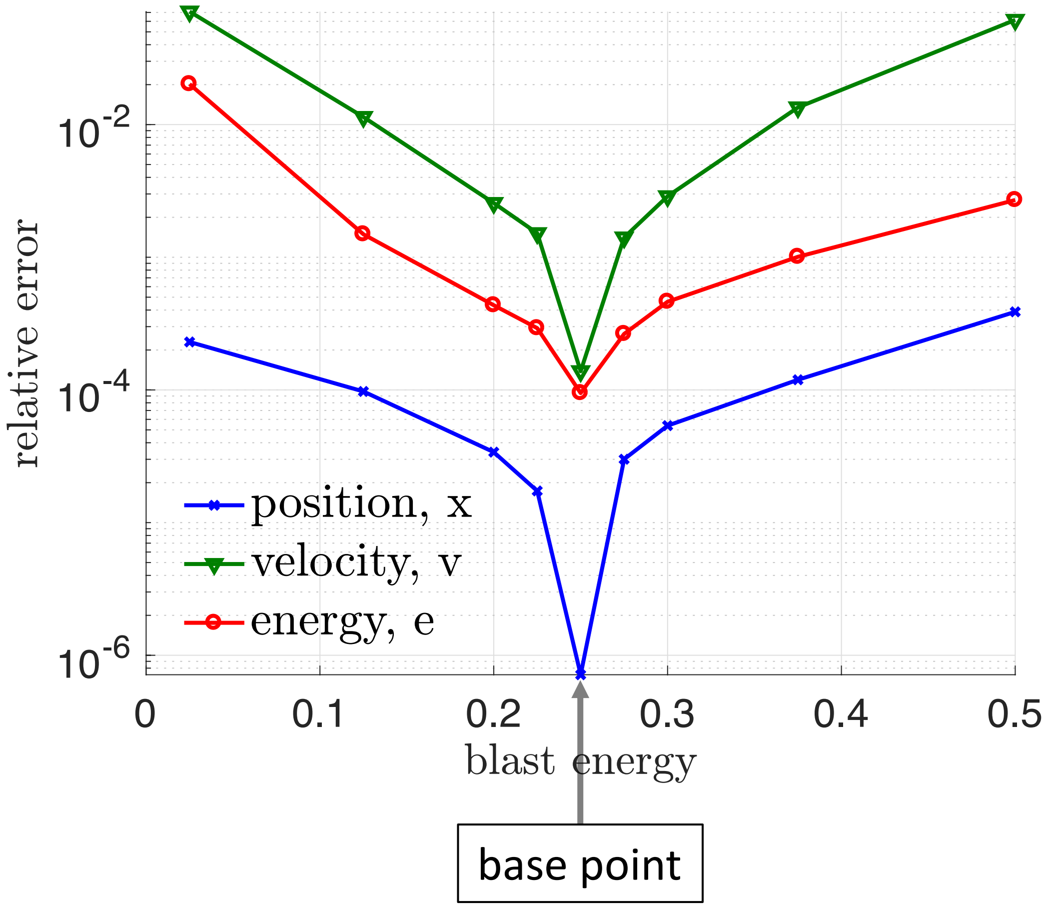




Kinematic dofs: 594
Energy dofs: 256

Kinematic dofs: 33,410
Energy dofs: 16,384

Robustness of a local ROM in extrapolation: Sedov blast



(Blast energy variation)

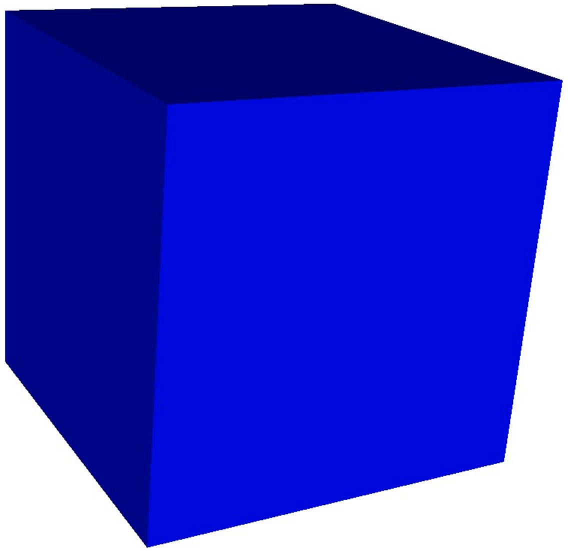
- Allows a fast gradient computation!
- Easy to increase the size of the parameter space

Greedy algorithm

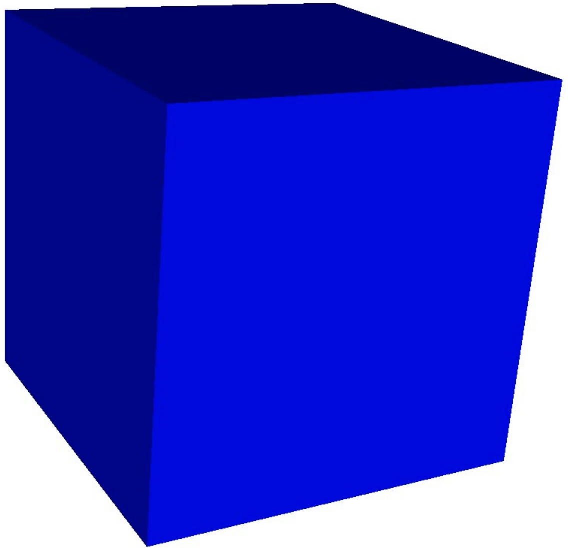
Goal: find an optimal set of local ROMs whose overall accuracy is less than 0.03.

Set parameter space: Blast energy [0.075, 1.25]

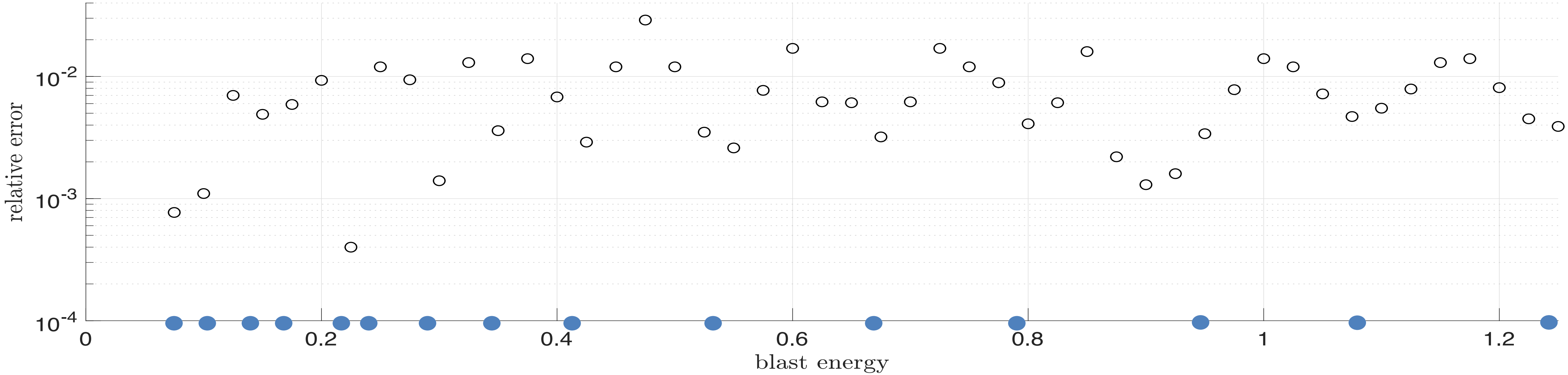
Error indicator: *cheap to compute but a good indicator for error measure*



Blast energy: 0.075



Blast energy: 1.25

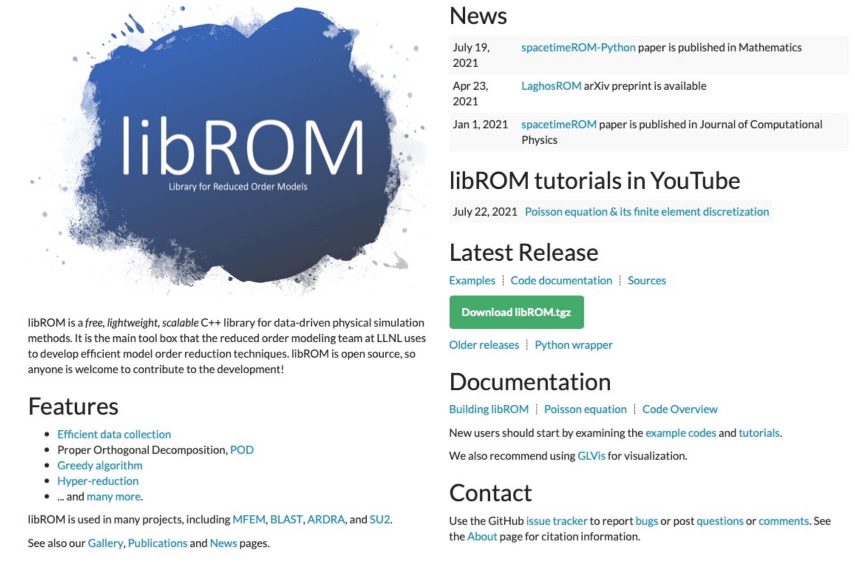


Linear subspace ROM for hydrodynamics

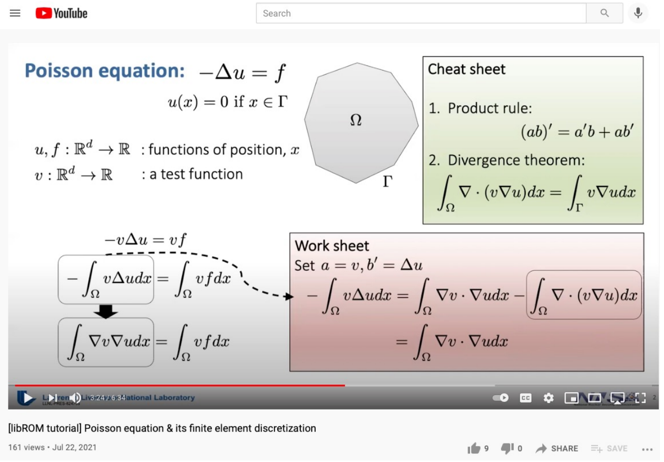
- **Paper**: Copeland, Cheung, Huynh, Choi, "Reduced order models for Lagrangian hydrodynamics" *arXiv preprint*, arXiv:2014.11404, 2021.

- **Software**:
  - libROM (library for reduced order models): https://github.com/LLNL/libROM
  - Laghos (physics solver for hydrodynamics): https://github.com/CEED/Laghos/tree/rom

- **Webpage** for libROM under construction

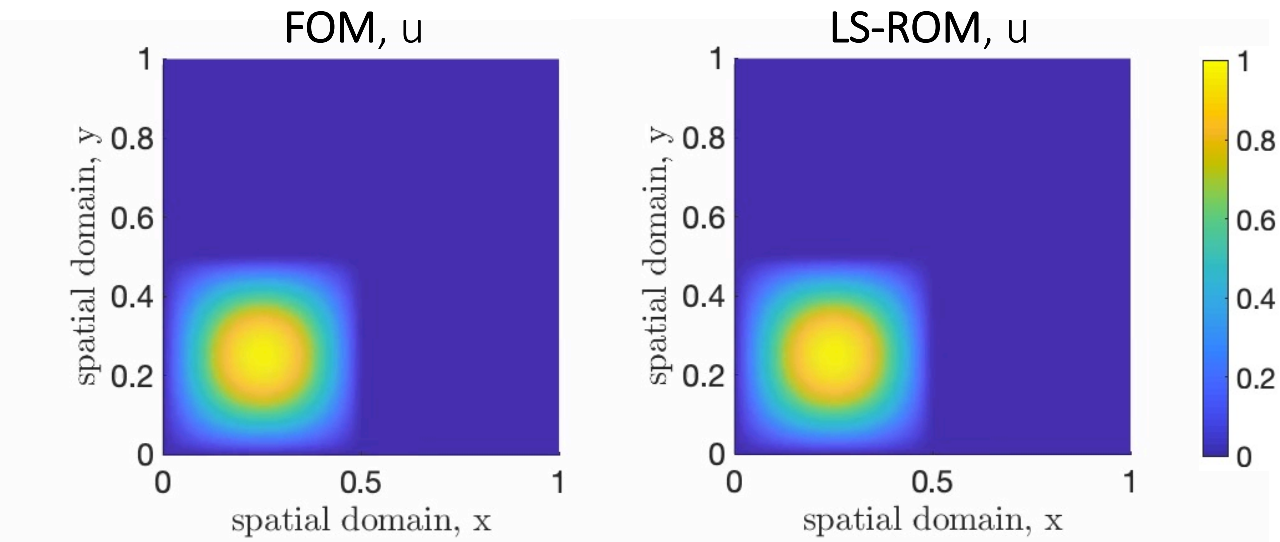


- libROM YouTube tutorial under production
  - https://youtu.be/YaZPtlbGay4



Numerical result: 2D viscous Burgers equation (advection-dominated)

$$\frac{\partial u}{dt} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \qquad \frac{\partial v}{dt} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \qquad Re = 1/\nu = 10,000$$



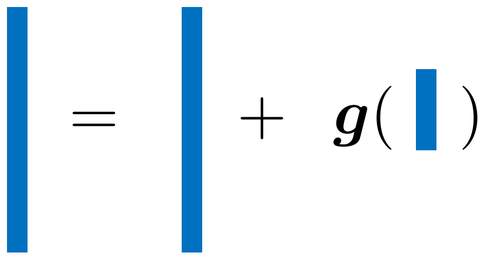
method	LS-ROM
max. rel. error (%)	34.4
speed-up	26.8

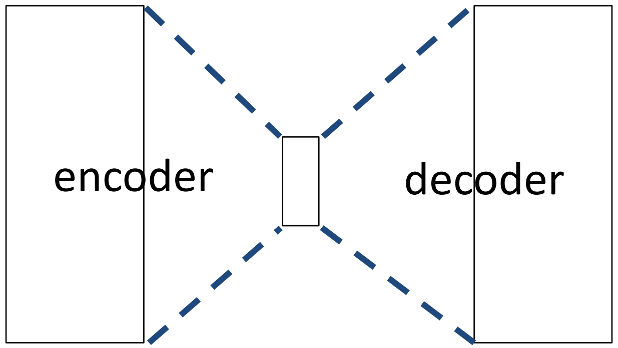
Nonlinear manifold reduced order models

Goal: exploit data to build nonlinear manifold solution representation that achieves ***much better accuracy and robustness*** than linear subspace-based reduced order model

- Governing equation: $\frac{d\boldsymbol{w}}{dt} = \boldsymbol{f}(\boldsymbol{w}, t; \boldsymbol{\mu}), \quad \boldsymbol{w}, \boldsymbol{f} \in \mathbb{R}^{N_s}$
- Solution approximation:

$$\boldsymbol{w} \approx \tilde{\boldsymbol{w}} = \boldsymbol{w}_{\text{ref}} + \boldsymbol{g}(\hat{\boldsymbol{w}}), \quad \hat{\boldsymbol{w}} \in \mathbb{R}^{n_s}, \quad n_s \ll N_s$$

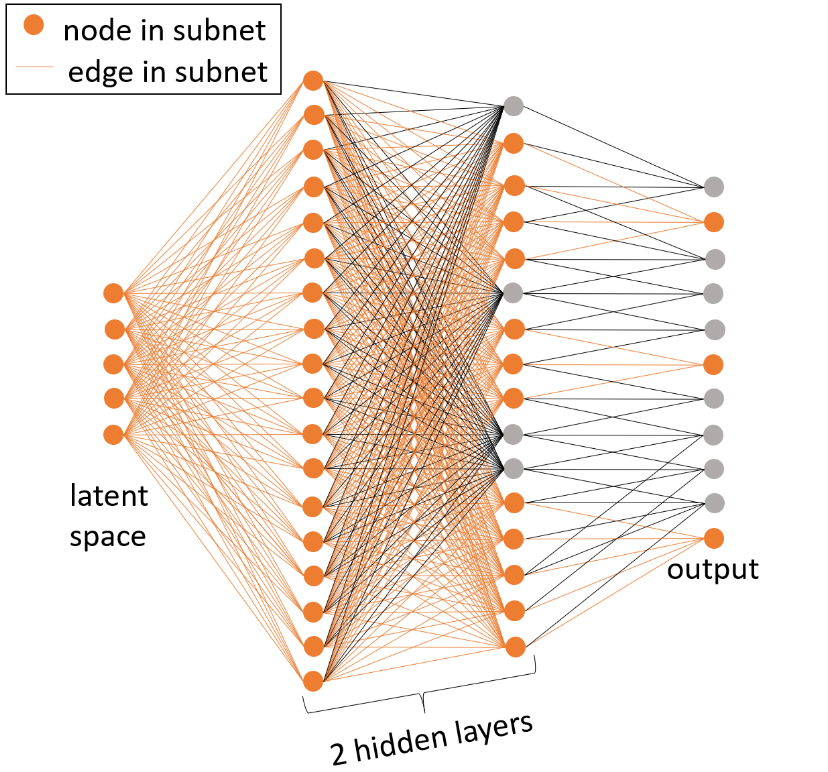


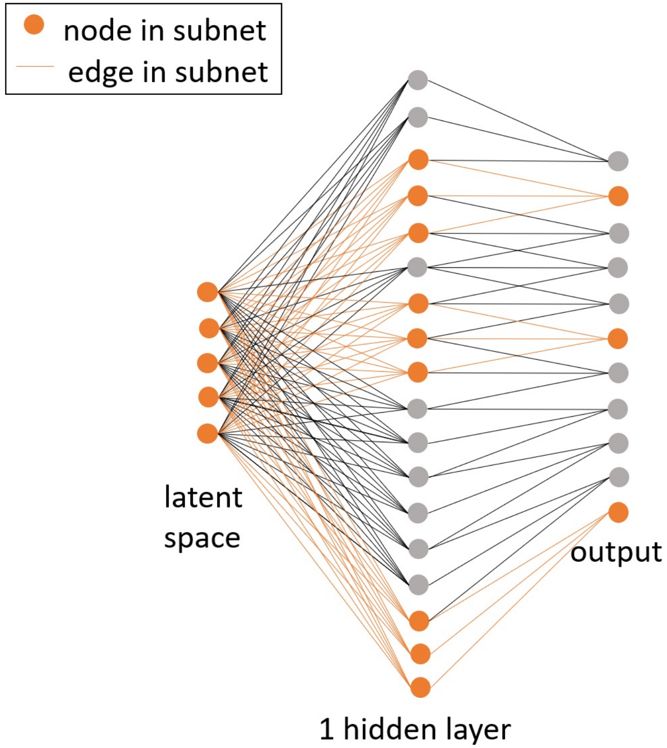


where $\boldsymbol{g} : \mathbb{R}^{n_s} \to \mathbb{R}^{N_s}$ defines a nonlinear manifold from reduced to full state

- The over-determined system: $\boldsymbol{J}_g(\hat{\boldsymbol{w}}) \frac{d\hat{\boldsymbol{w}}}{dt} = \boldsymbol{f}(\boldsymbol{w}_{ref} + \boldsymbol{g}(\hat{\boldsymbol{w}}), t; \boldsymbol{\mu})$ Hyper-reduction

Shallow vs. deep NN in the perspective of hyper-reduction



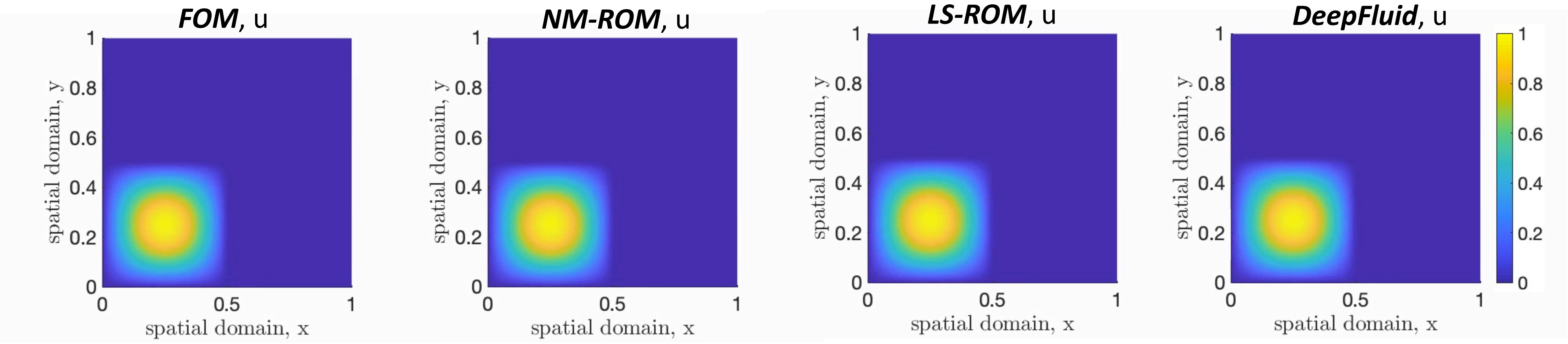


- A shallow neural network can provide sparser structure than a deep one in a subnet
- A sparse network is a key for successful NM-ROM hyper-reduction!

*Kim, Choi, Widemann, and Zohdi, ”A fast and accurate physics-informed neural network reduced order model with shallow masked autoencoder." *arXiv preprint, arXiv:2009.11990, 2020.*

Result: 2D viscous Burgers equation (advection-dominated)*

$$\frac{\partial u}{dt} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \qquad \frac{\partial v}{dt} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \qquad Re = 1/\nu = 10,000$$



method	NM-ROM	LS-ROM	BB
max. rel. error (%)	0.93	34.4	38.6
speed-up	11.6	26.8	119

*Kim, Choi, Widemann, and Zohdi, ”A fast and accurate physics-informed neural network reduced order model with shallow masked autoencoder." *arXiv preprint,* arXiv:2009.11990, 2020.

Summary

NM-ROM

solution dimension reduction

the existing numerical discretization

Machine learning

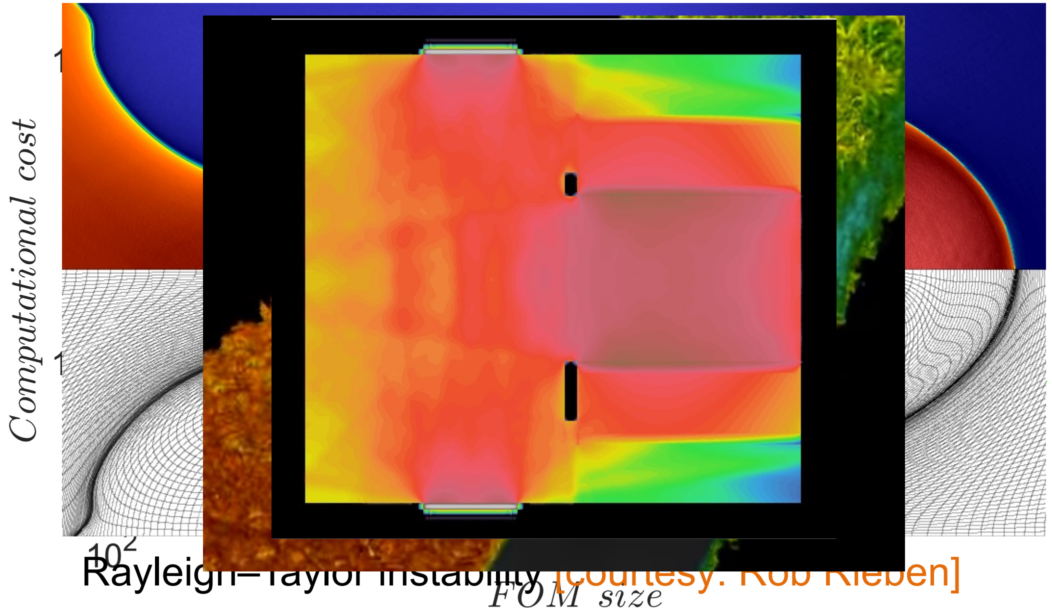
- Nonlinear manifold solution representation

Finite element, volume, difference methods

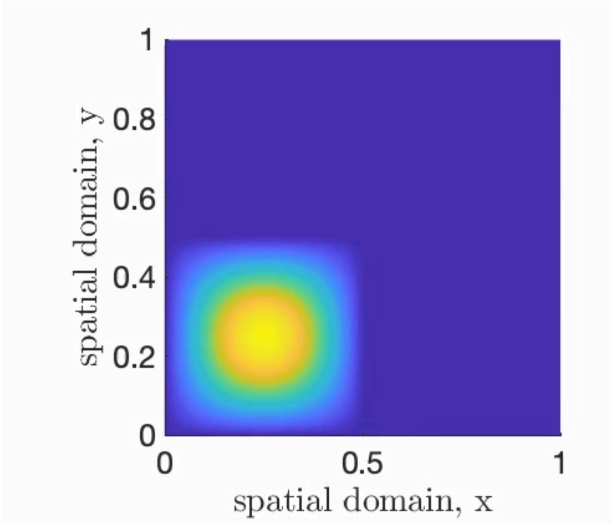
- Traditional solution process

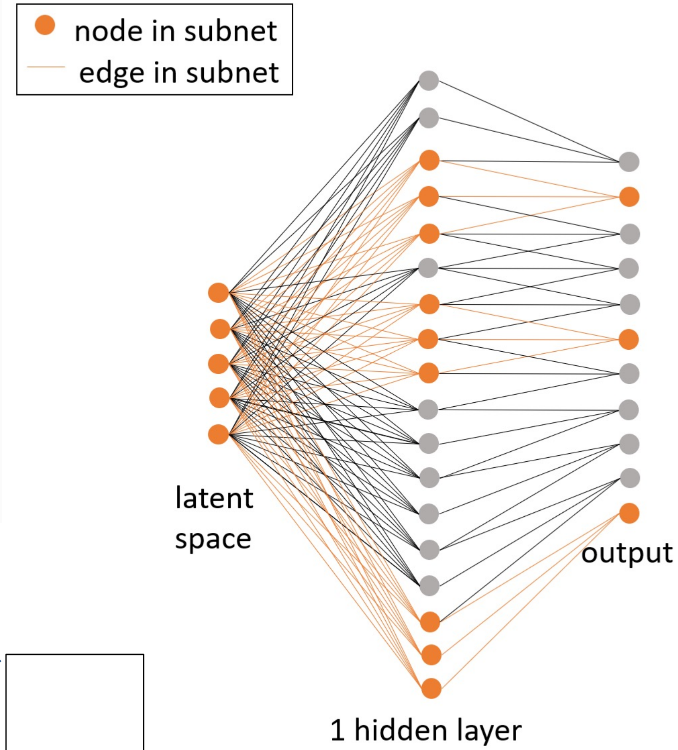
Future work

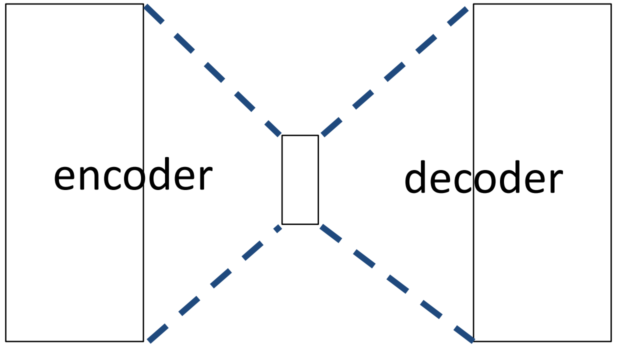
- ***NM-ROM*** for large-scale problems
- ***NM-ROM*** for mission critical problems, such as instability to turbulence, thermal radiative transfer, and shape charge simulations.

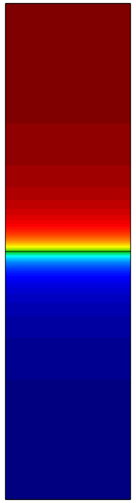


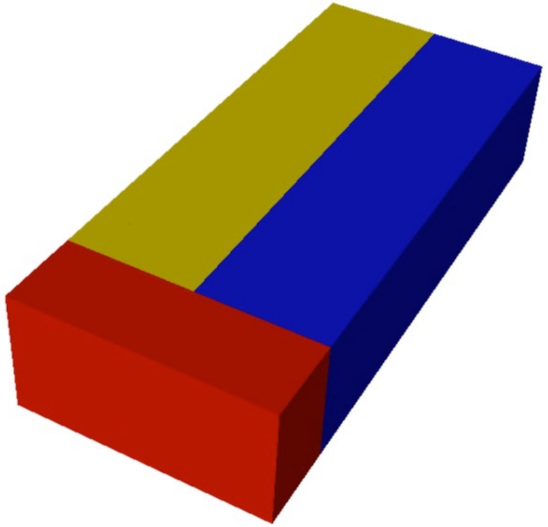
Questions? Email choi15@llnl.gov

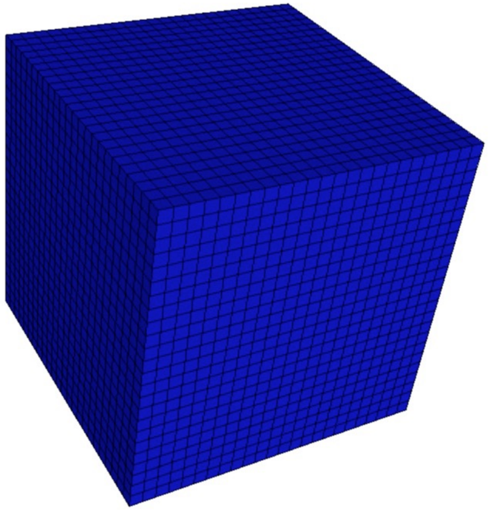


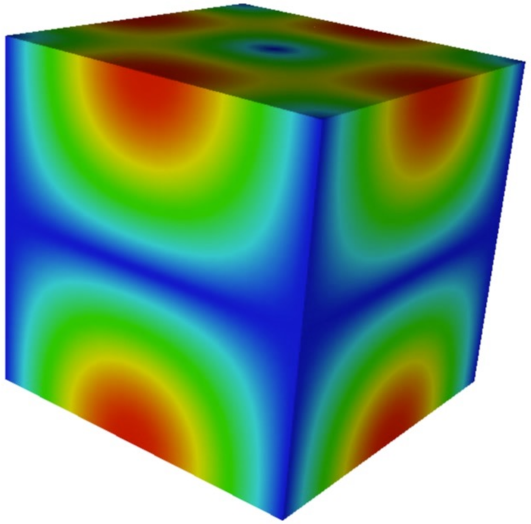












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